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Invited Review

25 years of DECOVALEX - Scientific advances and lessons learned from an international research collaboration in coupled subsurface processes

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ABSTRACT

This paper provides an overview of an international research collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems. The creation of the international DECOVALEX Project, now running for over 25 years, was initially motivated by the recognition that prediction of these coupled effects is an essential part of the performance and safety assessment of geologic disposal systems for radioactive waste and spent nuclear fuel. Later it was realized that these processes also play a critical role in other subsurface engineering activities, such as storage of CO_2, exploration of enhanced geothermal systems, and unconventional oil and gas production through hydraulic fracturing. Research teams from radioactive waste management organizations, national research institutes, regulatory agencies, universities, as well as industry and consulting groups have participated in the DECOVALEX Project, providing a wide range of perspectives and solutions to these complex problems. Analysis and comparative modeling of state-of-the-art field and laboratory experiments has been at the core of the collaborative work, with an increasing focus on characterizing uncertainty and blind prediction of experimental results. Over these 25 years, many of the major advances in this field of research have been made through DECOVALEX, as evidenced by three books, seven journal special issues, and a good number of seminal papers that have emerged from the DECOVALEX modeling work. Examples of specific research advances will be presented in this paper to illustrate the significant impact of DECOVALEX on the current state-of-the-art of understanding and modeling coupled THMC processes. These examples range from the modeling of large-scale in situ heater tests representing mock-ups of nuclear waste disposal tunnels, to studies of fluid flow and chemical-mechanical coupling in heterogeneous fractures, and to the numerical analysis of controlled-injection meso-scale fault slip experiments.

1. Introduction

1.1. Background

Coupled thermal-hydraulic-mechanical-chemical (THMC) processes in the deep subsurface refer to processes in geological formations at a depth of a few hundred meters or more, under the joint influence of thermal gradients, hydraulic pressure changes, rock mechanical stresses and geochemical reactions. Processes that occur include heat transfer and temperature variations, liquid and gas flows, rock mechanical deformation and fracturing, and chemical sorption, dissolution and precipitation. The term "coupled processes" implies that each process potentially affects and is affected by the initiation and progress of the other processes.[1,2] Thus, the response of a rock mass cannot be predicted with confidence by considering each process individually or in direct succession. In the field of rock mechanics and rock engineering, many studies have been made on binary couplings between TM and HM processes, but for a number of major geoengineering endeavors, it is

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[1] **In Memoriam** - This invited review paper is dedicated to the memory of our co-author and close friend John Hudson, eminent scientist in the field of rock mechanics and DECOVALEX Chairman from 2008 to 2015, who passed away unexpectedly on February 14, 2019.

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essential to understand and be able to model processes with THM coupling, and even full THMC coupling.

The present paper provides an overview of a long-term international research collaboration for advancing the understanding and modeling of coupled THMC processes in geological systems. The international collaboration, now running for over 25 years, is the DECOVALEX Project. It was initially motivated by the recognition that prediction of these coupled effects on potential transport of radionuclides from a subsurface repository of heat-releasing radioactive waste and spent nuclear fuel is an essential element of the performance and safety assessment of such a disposal system. But, later, it was realized that such coupled effects also play a critical role in a range of other sub-surface engineering activities, such as geological storage of carbon dioxide, creation and exploration of enhanced geothermal systems (EGS), and unconventional oil and gas production through hydraulic fracturing.

Society has imposed special demands on the safety assessment of geological disposal of radioactive waste not commonly encountered in geoengineering projects. Firstly, the time frame of prediction required in safety assessment typically reaches into hundreds of thousands of years and more. Secondly the evaluation of potential migration of radionuclides must consider very low concentration levels to conform to stringent international regulatory dose limits. Thirdly, a sufficient understanding of the key processes and their effects must be attained in order to provide confidence in the safety assessment.[3–5]

THMC processes have a critical input into the confidence building required to underpin safety assessments for most radioactive waste disposal concepts. Elements of demonstration of safety (often referred to as ‘safety functions’) can have very different constraints in terms of modeling requirements, evaluation confidence, and timescales. Numerical modeling of these safety functions can range from long-term whole-system type analyses for time periods of up to one million year (for example the performance assessment modeling of radionuclide transport from the repository to the biosphere to calculate dose/exposure) to detailed analyses of specific perturbations within a disposal facility which often occur during the first hundreds to thousands of years after repository construction (such as evaluation of excavation damage zone and changes in permeability, modeling of the early thermal transient and induced coupled processes, evaluation of seal performance etc.). Modeling laboratory and field experiments at different scales can help build confidence in process understanding to support long-term safety evaluations in general, but is considered particularly useful to answer key ‘questions’ posed by specific safety functions (and related impacts from early-time perturbations) via numerical prediction compared directly with experimental observation. Blind prediction of experimental outcomes can be the most powerful demonstration of confidence for a given aspect of a disposal facility or set of relevant coupled processes, but is also the most difficult logistically and practicality, given the incomplete constraints on even simple experiments. Evaluation of the limited effects of such incomplete constraints can probably be considered as part of the confidence demonstration.

It was with this background that the need for improving our understanding and modeling of coupled THM and THMC processes was recognized and the DECOVALEX Project was initiated.

1.2. Modeling THMC processes: approaches, complexities, and uncertainties

For the performance assessment of a radioactive waste repository, model analyses of coupled THMC effects has to account for, either implicitly or explicitly, heat release from the waste, rock mechanical changes due to repository excavation, as well as changes in water pressure and chemical reactions that affect water and gas flow paths and contaminant transport characteristics (Fig. 1). Many of the modelled processes are non-linear and the constitutive relationships between them are not well known. Often alternative constitutive relationships exist, with the different alternatives suitable for different

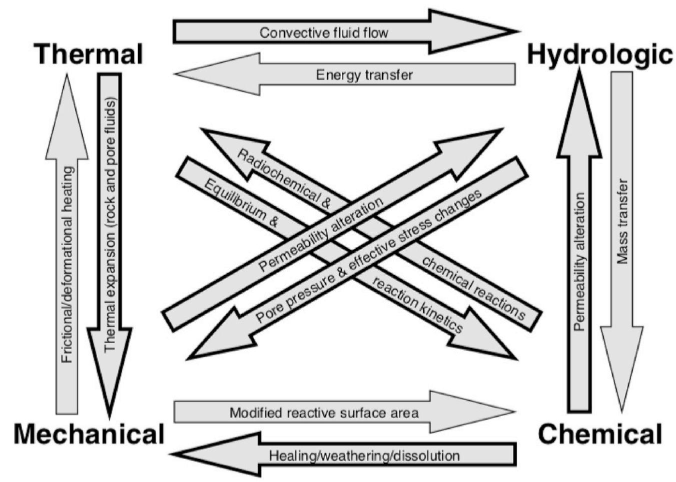


Fig. 1. Coupled thermal-hydraulic-mechanical-chemical effects in nuclear waste isolation. Bold arrows emphasize interactions that are of potentially greater performance significance (From Yow and Hunt[8]).

geological settings. However, details of the geological settings and site characteristics cannot be known completely due to practical limitations on site observations and field tests. The appropriate level of necessary site measurements is a question which modeling is often asked to help to answer, and regions of the site where measurements are sparse would have to be represented by some average or representative characteristics. Thus, coupled THMC modeling of geological processes is a complex and challenging task.

Not all coupled processes occurring in a geological formation need to be represented explicitly in a simulation model. Some may have small impacts even for predictions into thousands of years and can be ignored. Others may be “lumped” with one another by the use of effective parameters. What are the major coupled THMC processes to include and what effective parameters can be employed in a simulation model depend on the specific safety criteria, scenarios and site characteristics.

As can be seen from the discussion above, there are many choices research groups have to make in performing modeling studies of coupled THMC processes, such as selection of processes to be included, choice of constitutive relationships, representation of areas with sparse data, definition of boundary conditions and model properties, and use of alternative numerical techniques. Model comparison studies by multiple research groups using different approaches are very useful for understanding the uncertainties arising from such conceptual model choices. In this context, a method of evaluating the confidence level of model outcomes needs to be developed.

The uncertainty arising from conceptual model approaches is not unique to radioactive waste repository performance assessment. It is also found, for example, in the field of geological carbon storage, where it is important to understand the underlying physical and chemical processes that control the movement of CO_2 in the subsurface. Mukhopadhyay et al.[6] point out that, while building conceptual models for these complex and often coupled processes, modelers make various choices regarding implementation of multiphase behavior of the fluids and their equations of state, approaches for coupling of processes, modeling techniques, and selection/interpretation of site characterization and monitoring data. These model choices often lead to a wide range in system evolution, even if each of the models is considering the same operation scenario at the same CO_2 storage site. This may be termed as model uncertainty, which is one of the greatest sources of uncertainty and risk for predictive modeling.[7]

The various sources of uncertainty lead to the realization of the crucial role of validating model results against laboratory and field data. In the field of radioactive waste repository safety assessment, many laboratory experiments have been designed and carried out using small core samples as well as large rock samples with sizes up to about 1 m in diameter. Field measurements and field tests are also conducted on experimental sites, some of which in locations where repositories have been proposed to be situated and others in suitable areas with representative geologic conditions. A number of underground research laboratories (URL) have been constructed in major countries as specific dedicated facilities to conduct tests to investigate various concepts, study processes and check modeling results,[9] often at the spatial scale envisioned for the ultimate waste emplacement in subsurface tunnels. Experimental work, be it in the laboratory or in the field, is mainly conducted for a particular scenario under particular well-defined driving forces such as changes in stress, pressure or temperature gradients. Numerical simulations with different modeling approaches are then performed to test particular aspects in the capability of the model against measured data, which if successful provides confidence in the evaluations made for safety and performance assessments. The goal is not only to improve model approaches and increase model confidence, but also to allow an estimate of uncertainty ranges. It is to be noted that acquiring the necessary field data—in underground research facilities or other field measurement campaigns—is typically a major multi-year undertaking which requires major national financial resources.[10,11]

1.3. The DECOVALEX project

Recognizing the need for a deeper understanding of coupled THM and THMC processes and development of modeling techniques, as well as the importance of model comparison and testing against laboratory and field data by multiple teams using multiple approaches to estimate uncertainty ranges and to enhance confidence of model results, the DECOVALEX Project was initiated in 1992 (www.decovalex.org). It is an international cooperative project of primarily nuclear waste management organizations, including implementers, regulators, and research institutes involved in national programs (from Switzerland, Japan, Canada, France, Czech Republic, Sweden, United Kingdom, Finland, China, Korea, Germany, Spain, Taiwan and the United States), plus a large number of associated modeling teams. Under this project, the research teams have been able to share and study data from major and expensive laboratory and field experiments. In-depth and detailed discussions among the teams have yielded insight into the coupled THMC processes and have stimulated development of modeling capabilities and measurement methods which would not have been possible if the data had been studied by only one or two groups.

Since the project initiation, the project has been operating in several four-year phases, each phase featuring a small number (typically three to seven) modeling tasks of importance to radioactive waste disposal, together covering a large number of theoretical, numerical, laboratory and field studies. Six project phases were successfully concluded between 1992 and 2015, results of which have been summarized in several overview publications[12–14] and described in detail in a series of Special Issues in the International Journal of Rock Mechanics and Mining Sciences (Vol. 32 (5) in 1995, Vol. 38 (1) in 2001, and Vol. 42 (5–6) in 2005), in the Journal of Environmental Geology (Vol. 57 (6) in 2009), in the Journal of Rock Mechanics and Geotechnical Engineering (Vol. 5 (1–2), in 2013), and in a 2018 Topical Collection "DECOVALEX-2015" in the Journal of Environmental Earth Sciences. The current phase, named DECOVALEX-2019, runs from 2016 through 2019. Over the past two and a half decades, during which the project has made significant advances in modeling THM and THMC, its main objectives have not changed:

- To support development of numerical simulators for THM and THMC processes in geological systems
- To investigate and implement suitable algorithms for THM and THMC modeling
- To compare model calculations with results from field and laboratory experiments
- To design new experiments to support code and model development
- To study the application of THM and THMC modeling to performance and safety assessment of nuclear waste repositories

One of the most important characteristics of DECOVALEX is the emphasis on in-depth interaction between the research teams and on a cooperative supportive environment. Scientific workshops are held twice per year, and task-specific discussions may be held in between. At the workshops, detailed discussions allow for efficient exchange of information and sharing of scientific knowledge. Through comparisons of results from the research teams, much insight is gained, not only on the effects of coupled processes, but also on the strengths, weaknesses, and adequacies of the various approaches and computer codes. It is also an effective way for participants to learn from each other and for new research teams, graduate students and early-career researchers to get up to speed on the state of art in this research field.

2. DECOVALEX setup and activities

From the onset, the organization for the DECOVALEX Project was set up as simple and as effective as possible. The project consists of a number of organizations from different countries, called the funding organizations, who jointly support the project (for a given four-year project phase) and provide funding to their own research team (or teams) working on the tasks defined in the project. Representatives from the funding organizations form a Steering Committee to direct all project activities. The Steering Committee is assisted by one selected funding organization for managing all administrative matters (the managing participant), a chairman for providing general scientific direction and guidance in defining project tasks, and a technical coordinator for handling all technical and reporting matters. Through the Steering Committee and close communication among the managing participant, committee chairman and technical coordinator, the project can be run in a very efficient and flexible way. This is demonstrated by the fact that DECOVALEX has been successful to continue phase after phase over the last 25+ years. Appendix A shows a list of funding organizations and research teams over the project phases from 1992 to today.

At the start of the project in 1992, the Steering Committee decided to define the project activities as studying a number of benchmark tests (BMT) and test cases (TC) of importance to radioactive waste disposal and other subsurface engineering applications. The BMTs investigate hypothetical problems in the behavior of individual or multiple coupled THM and THMC processes, and in some cases analyze the extrapolation of results over the large temporal and spatial scales of interest to repository performance. The TCs are actual laboratory and field experiments studied and modelled to advance our understanding of the THM and THMC processes based on measured data. This dual-prong strategy has been followed throughout the duration of the project to date. A number of large-scale, multiyear field experiments have been analyzed within the project, such as the Kamaishi THM Experiment, the FEBEX experiment in Grimsel underground research laboratory, and the Yucca Mountain drift scale heater test (DST) which was at a site proposed for a repository at that time. Appendix B shows a list of major BMTs and TCs which have been studied over the project phases from 1992 to today.

BMTs and TCs are collectively modelled by DECOVALEX participants. As modeling teams provide their individual results for the same modeling challenge, comparative assessment can assist both to interpret and understand the experimental results and to test the simulation models used. While code verification and benchmarking efforts have been undertaken elsewhere to test simulation codes,[15,16] the model comparison conducted within the DECOVALEX framework is different because (a) the modeling tasks are often actual laboratory and field experiments, and (b) DECOVALEX engages model comparison in a broad and comprehensive sense, including the modelers' interpretation of experimental data, selection of boundary conditions, rock and fluid properties, etc., in addition to their choice of coupling schemes and simulators. Based on the results from such broad model comparison, key data needs can be identified, new model capability developments may be undertaken and new experiments be proposed to advance the state of mathematical modeling for coupled processes in geological systems.

3. Project progression through successive DECOVALEX phases

One of the principles of DECOVALEX is that in each project phase the portfolio of modeling tasks is defined collectively by project participants, in a process where TC's and BMT's proposed by some funding organizations are selected based on the interest of other project partners to engage in them as a participating modeling team. Thus, the tasks selected over the 25 years of DECOVALEX existence mimic closely the broader evolution of the scientific issues of importance in the field of radioactive waste disposal. We provide below a brief review of these trends—in terms of host rock preference, emphasis of engineered versus natural barrier, importance of various coupled processes, spatial and temporal scale, as well as numerical methods used—and in Sections 4 and 5 illustrate these further by giving summaries of several selected DECOVALEX tasks.

3.1. Key processes, repository stages, and host rock characteristics

To provide a general framework for discussing coupled processes and their relevance, it may be worthwhile to introduce distinct periods in the development of a geological repository for radioactive waste (see Fig. 2). Tsang et al.[17] contrasted the key processes and issues in early repository implementation phases (Construction and Open Drift Stage) with those occurring during a period of thermal disturbance after waste emplacement (Exploitation Stage) and during a long-term period where much of the early perturbations are starting to subside and the system is approaching a late time equilibrium (Long-Term Post-Closure Stage).

Key processes in the early stages of repository development are the potential creation of an excavation damaged zone (EDZ) of increased permeability around the tunnels. Performance assessment requires knowledge about how EDZ properties evolve over time and, in the case of clay repositories, how they may be affected by tunnel ventilation and saturation changes. During the Exploitation Stage, decay heat from radioactive waste may generate large temperature increases in the buffer and the near-field rock, while at the same time resaturation of the near field occurs as a slow process governed by relatively low rock permeability and buffer characteristics. Heating may lead to water vapor convection near the heat sources and generate transient pore-pressure buildup resulting from differential thermal expansion, leading to changes in effective stress state in the engineered and natural barrier system. Heating may also affect important rock properties such as rock strength, and may induce chemical reactions with impact on rock properties.

The Long-Term Post-Closure Stage is the basic period of concern for long-term performance and safety assessment because it is the most likely stage when failure of the engineered barriers may occur and lead to the release and subsequent transport of radionuclides and any non-radioactive contaminants. The transport characteristics in the tunnel backfill and near-field rock during this period depend strongly on the coupled processes and effects that occurred during the previous stages. In addition, there are some long-term coupled processes during this stage that can potentially affect radionuclide migration, such as geochemical processes or gas production from the degradation of repository engineering materials. And finally, this long-term period is also concerned with radionuclide transport in the rock mass away from the repository, which is strongly affected by the host rock characteristics and heterogeneities as well as coupled THMC processes associated long-term climate variations.

Over the 25 years, the DECOVALEX Project has tackled a variety of the key processes mentioned above, with an emphasis on the perturbations occurring during the earlier repository stages, and it has done so for most of the major rock types considered for hosting geologic repositories (crystalline rock, sedimentary rock, indurated clays, plastic clays, and rock salt). While there are considerable differences between rock types with regards to the key processes affecting repository safety, there are also many similarities, and the concepts, experimental approaches, and numerical models are often transferable.[19] Within DECOVALEX phases, the consideration of key processes has often been done simultaneously for a variety of rock types, which in turn have helped provide deeper insight and higher confidence in our understanding of any one particular rock type of interest.

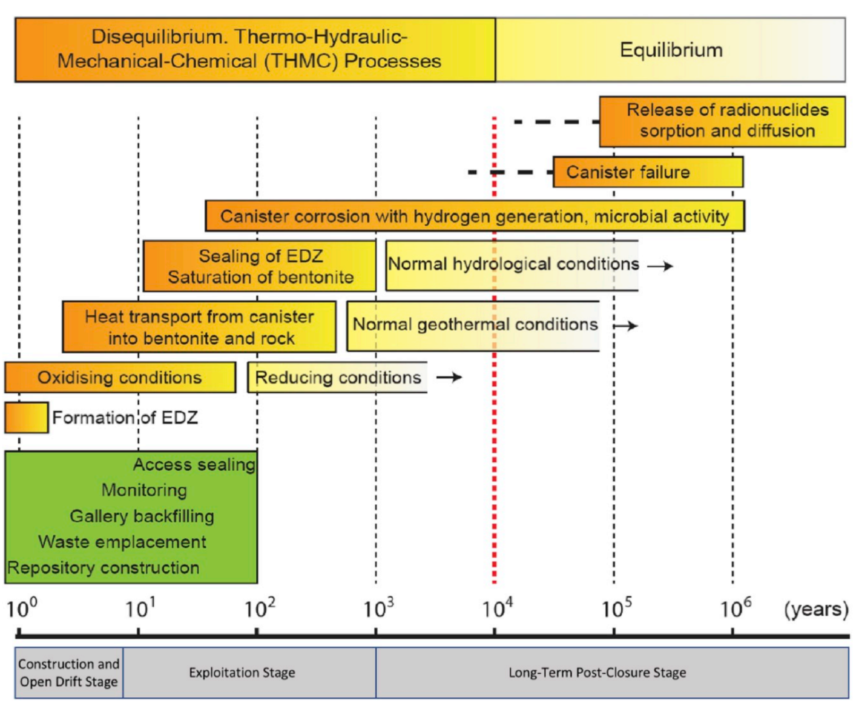


Fig. 2. Schematic showing the relevant processes occurring during the lifespan of a repository are given in light red, starting with the formation of the excavation damaged zone (EDZ) and ending with the release of radionuclides from breached canisters, based on the Swiss disposal concept as an example. Indicated in green are the human engineering activities starting with the construction of a repository until its sealing at the end (the time periods are best estimates) (Adapted from Bossart et al.[18]). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

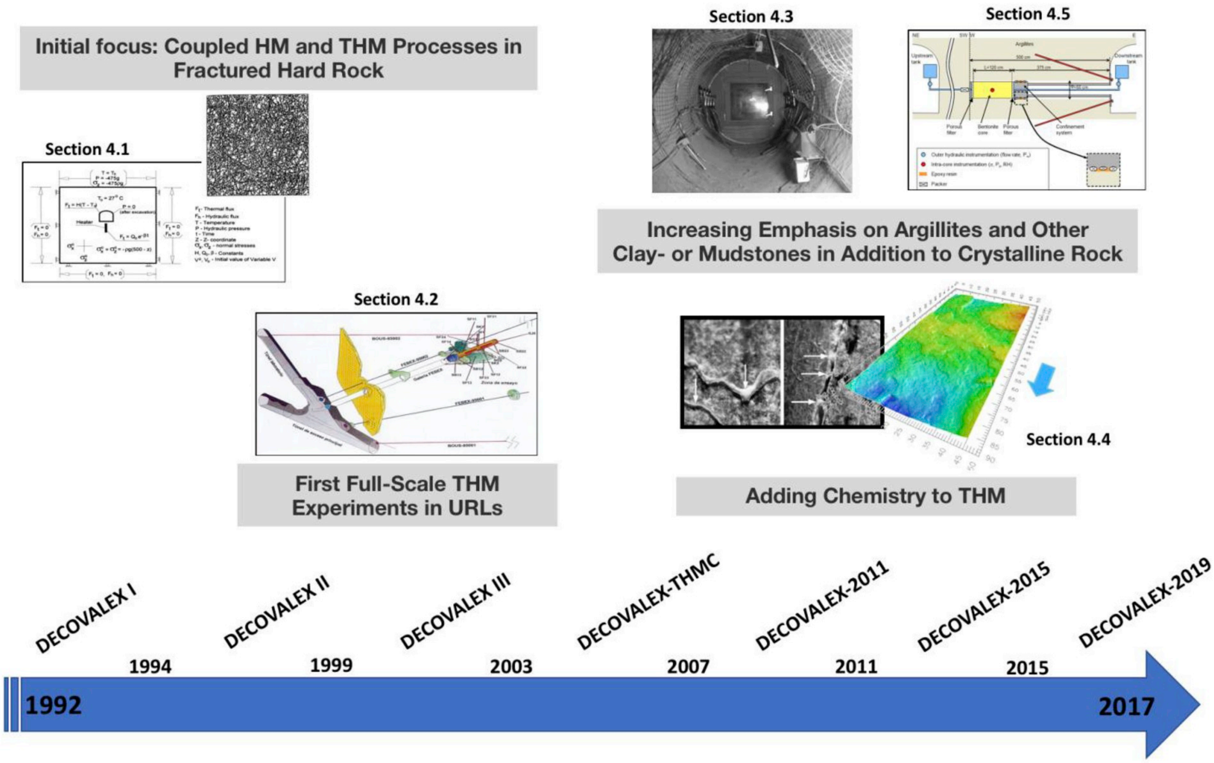


Fig. 3. Simplified evolution of important research areas in the DECOVALEX Project. Embedded graphics illustrate the five selected task examples described in Section 4, each representative of major DECOVALEX achievements.

3.2. DECOVALEX evolution through 25 years

This section gives a brief review of research highlights illustrating the philosophy of the DECOVALEX Project and some major trends observed over the course of 25 years. Fig. 3 places five modeling tasks, each selected as examples for the scientific evolution of the project, onto a DECOVALEX timeline from 1992 to 2017.

In 1992 when DECOVALEX was founded and in the following decade, many nuclear-energy nations worldwide focused on hard competent crystalline rock like granite to host a waste repository.[20,21] Most of these countries participated in DECOVALEX as partner organizations (e.g., France, Canada, Spain, Japan, United Kingdom, Sweden, and Finland). It is therefore no surprise that many of the test cases and benchmark tests during the first three phases of DECOVALEX (I, II and III) addressed coupled THM processes in crystalline rock with focus on the multiple fractures in such rocks since the fractures provide the main pathways for flow and solute transport. In a few cases, the role of bentonite backfill as an important engineered barrier in such rocks was also investigated.

At the time of these DECOVALEX phases, scientists were just starting to experiment with different conceptual approaches and simulation methods to model thermally-driven coupled flow and mechanics in fractured rock. This is reflected in the task portfolio in DECOVALEX I, which focused on basic process understanding and development of constitutive relationships. Research teams worked on (1) three benchmark tests comparing a range of simulation approaches for HM and THM processes in well-defined fracture-matrix systems, (2) three small laboratory experiments to improve fundamental relationships between the permeability of fractures and shear versus confining pressure, and (3) two small-scale field tests addressing the role of coupled hydro-mechanical processes. One of the benchmark tests from DECOVALEX I, BMT3, is further described in Section 4.1 as a good example of a synthetic task testing the capabilities of many alternative conceptual models and computer codes. The task features a representative emplacement design with a tunnel and heated deposition hole embedded in a fractured crystalline host rock system with thousands of explicitly defined fractures. The modeling teams used a range of approaches ranging from continuum to hybrid to discrete fracture methods to simulate the THM processes occurring during excavation and waste emplacement, collectively providing a much clearer understanding of conceptual model uncertainties arising from the use of different constitutive relationships, homogenization techniques, degrees of simplification, and numerical solution methods.

The progression from DECOVALEX I to DECOVALEX II and III corresponds to continuing advances in the research field of coupled THM process modeling. While DECOVALEX I represented an initial stage of such research investigation involving a number of laboratory and small-scale field investigations, DECOVALEX II focused on comprehensive studies of two field tests in Japan and in the United Kingdom. The trend to larger and more complex field studies continued in DECOVALEX III, which was motivated by two of the most important multi-year thermal experiments available to date, the Full-scale Engineered Barrier Experiment (FEBEX) with bentonite-backfilled tunnels in crystalline rock at the Grimsel Test Site in Switzerland and the Drift Scale Test with an open-drift concept in volcanic tuff at Yucca Mountain in the United States. Both experiments were full-scale realistic representations of a waste emplacement tunnel featuring the repository concepts envisioned in the mid 90's by the Spanish and the U.S. programs. Modeling teams involved in either experiment gained an integrated perspective of the behavior of disposal concepts in fractured crystalline rock and fractured volcanic tuff. The monitoring data provided to the teams proved invaluable for verifying, validating and studying the capabilities of a number of numerical codes held by the DECOVALEX III project teams. More detail on the FEBEX test is given in Section 4.2.

In 2004, the progression into its fourth phase, referred to as DECOVALEX-THMC, marked an important refocusing and expansion of the collaborative research project, in terms of processes addressed and host rocks studied. DECOVALEX-THMC involved a first push to adding chemistry (or "C") to the primarily THM coupling in previous phases. One modeling task looked into the impact of temperature-induced precipitation and dissolution on the porosity and permeability of the host rock in the near field of a repository, in volcanic and crystalline-bentonite systems. At the same time, DECOVALEX-THMC moved beyond the crystalline rock cases in response to some major nuclear energy nations starting to research disposal in argillaceous clays (e.g., France, Switzerland,[22]), and for the first time DECOVALEX included a test case featuring a rock characterization experiment in an argillite URL (the Tournemire site in France). This phase thus investigated three alternative rock types simultaneously, crystalline rock, volcanic tuff and argillaceous clay. It is also worth noting that four of the five DECOVALEX-THMC tasks were related to coupled phenomena in the near-field, and in particular the processes defining the creation and evolution of excavation damaged zones (EDZ).

Moving into DECOVALEX-2011, the fifth project phase from 2008 through 2011, we see a continuing trend with increasing emphasis on argillite host rocks and coupled chemical reactions. For example, Task A of DECOVALEX-2011 featured a large-scale experiment conducted from 2002 through 2006 in a 10 m long micro-tunnel at the Mont Terri URL in Switzerland referred to as Ventilation Experiment, or VE. This experiment examined the hydro-mechanical and chemical changes that may occur in argillaceous host rocks, especially in relation to the coupling with the ventilation of drifts and the cyclic desaturation of the near-drift host rock (see details in Section 4.3). At the same time, several DECOVALEX partner organizations maintained their focus on crystalline disposal environments, which explains the continuing study of emerging research issues relevant to crystalline rocks within the task portfolio.

DECOVALEX-2015 is the most recent phase that was fully completed at the time of writing this article. Chemical processes are now ingrained in many of the tasks conducted. A prime example is Task C1, which pushed the state of the art of modeling the fully coupled THMC interactions occurring in a single rock fracture exposed to fluid flow and reactions, heat, and confining stress (see Section 4.4). This sixth project phase also saw an increasing emphasis on buffer and sealing materials and their system performance in conjunction with the natural barrier. For example, two heater test tasks, based on large-scale experiments in the Mont Terri URL Switzerland and in the Horonobe URL, Japan respectively, explored the THM and THMC processes occurring in disposal tunnels with bentonite backfill embedded in a clay or mudstone host rock. In addition, the SEALEX Experiment in the Tournemire URL studied the barrier performance of the tunnel seals required in geologic repositories and how these are affected by HM couplings during bentonite hydration and swelling (Section 4.5). As a good example of a task structured into a sequence of simple to complex modeling steps, research teams were asked to work through preparatory steps of increasing complexity, starting with the simulation of laboratory and mock-up tests and separate responses of seal material versus host rock, before focusing on the integrated system behavior of the in-situ SEALEX Experiment.

Currently, the DECOVALEX Project is in the middle of its seventh phase, referred to as DECOVALEX-2019. The characteristics and trends that have shaped the first six phases are reflected in the current task portfolio, this time featuring a record number of tasks (seven) and a near-record number of funding organizations (13). In the task list in Appendix B, we see that this phase includes even coupling to biological processes. We also see not only a balance between different host rocks as well as between engineered and natural barriers involving a broad range of scales both in space and time, but also a mix of fundamental research tackling the basic understanding of complex processes versus more applied tasks looking into integrated behavior of disposal systems and sub-systems.

To provide a brief overview of on-going activities, we have selected three representative DECOVALEX-2019 tasks in Section 5 where more detail is provided. The first task explores an emerging concern in the nuclear waste community about gases produced from the corrosion of engineered barrier materials and whether, in low-permeability elasto-plastic materials such as bentonite and clay, they can move away from their source without creating overpressure and rock damage (Section 5.1). The second task is about progressive upscaling of THM processes from core experiments in the laboratory to small-scale field experiments (some cubic meters) to real scale disposal systems (entire tunnel segments) and to the scale of an entire waste repository (cubic kilometers) (Section 5.2). The third task addresses important issues related to the potential creation of flow paths for contaminant transport in otherwise low permeability argillaceous rocks (Section 5.3). Such flow paths could be created by reactivating faults of various sizes by thermal, hydraulic or mechanical disturbance during the operational and post-closure stages of a repository. The modeling challenge is based on a recent fault activation experiment performed at the Mont Terri URL, featuring controlled fluid injection directly into different fault compartments and measuring the hydromechanical response as a function of time.

It is interesting to note that all three tasks described in Section 5 are relevant beyond just radioactive waste disposal, meaning that experience gained through them is of direct relevance to other subsurface engineering applications such as geologic carbon sequestration, geothermal energy production, unconventional oil and gas production, waste water disposal, energy storage and gas storage. The DECOVALEX Project recently felt that there might be an opportunity for mutual benefit by bringing broader subsurface science expertise to bear on these data sets. As a first step in this direction, the Steering Committee decided to open up the fault reactivation task by inviting participation from organizations not traditionally part of DECOVALEX or the radioactive waste disposal science community.

4. Example tasks and lessons learned

Here we present selected examples of past modeling tasks conducted within the DECOVALEX Project, together conveying the topical breadth of the activities as well as the unique characteristic of in-depth collaboration between international researchers of different disciplines using a range of different approaches.

4.1. Benchmark test 3 (DECOVALEX I)

Benchmark Test 3 (BMT3) was conducted during the first DECOVALEX phase and became one of the "classical" DECOVALEX tasks, a good example for testing collaboratively the capabilities of many alternative models and computer codes.[23] The problem is associated with a near-field repository model, set up as a two-dimensional plane-strain problem in which a tunnel with a deposition hole is located in a fractured rock mass. The model domain is a 50 m by 50 m vertical cross section, situated 500 m below ground level (Fig. 4a). The modeling task is set up as a fully coupled THM near-field repository problem, with thermal effects caused by heat released from radioactive waste in the deposition hole (the heater). Heat output decreases exponentially with time. The crystalline rock mass surrounding the hole features a dense fracture network with a two-dimensional realization of 6580 fractures, built from a realistic three-dimensional fracture network model of the Stripa Mine, Sweden. The rock matrix is assumed to be isotropic and linearly elastic, with mechanical properties assumed independent of temperature variations, and thermal conductivity and expansion. The fractures are defined as parallel, planar, smooth surfaces with an effective hydraulic aperture. The initial and boundary conditions for the mechanical, thermal, and hydraulic effects are shown in Fig. 4a, with heating maintained for 100 years.

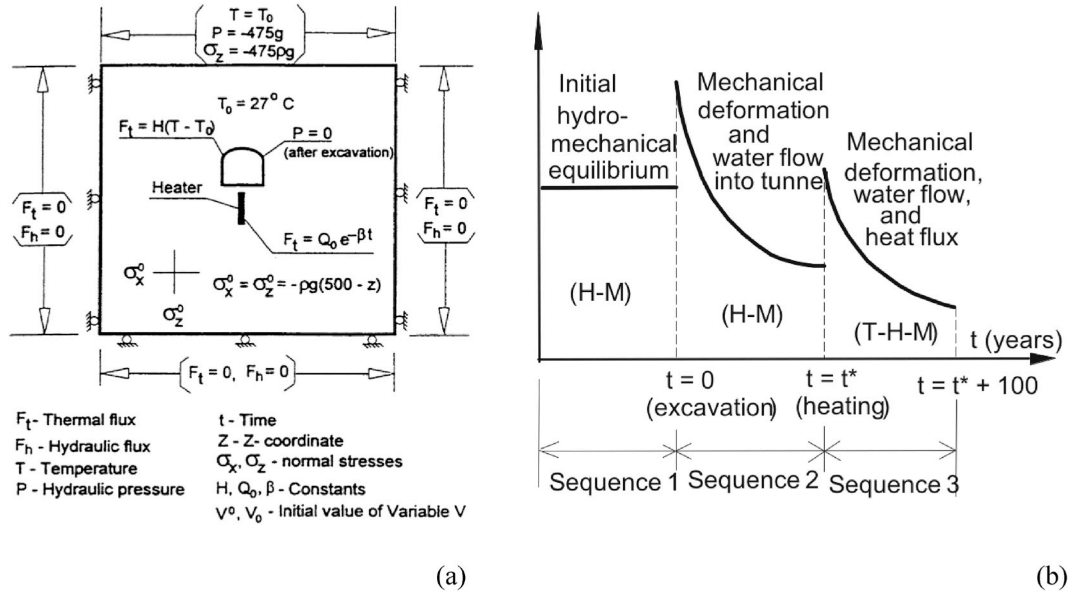


Fig. 4. (a) Model geometry and boundary conditions of BMT3, and (b) modeling sequence with repository stages (From Stephansson et al.[23]).

Three modeling stages were simulated in BMT3, see Fig. 4b. Stage 1 is the loading of the computational model prior to excavation of the tunnel under initial and boundary conditions of hydro-mechanical effects. An initial hydro-mechanical equilibrium should be achieved at the end of this loading stage. Stage 2 is the excavation of the tunnel, executed at the end of Stage 1. The initial hydro-mechanical equilibrium is disturbed and a new HM equilibrium should be achieved at the end of this stage, denoted as time $t = t^*$. Stage 3 begins the thermal loading, starting at time $t = t^*$ and maintained for 100 years.

The problem was studied by eight research teams. Fig. 5 shows the different representations and simplifications in the models used by the various teams. The studies produced insight not only into the effects of coupled THM processes, but also into the uncertainty and confidence levels of numerical simulations of these processes. As representative examples of the results obtained, Fig. 6 shows distributions of the stress (horizontal component) and temperature along a vertical profile cutting through the tunnel center, and Fig. 7 shows the water flux into the tunnel across its perimeter, produced by multiple research teams using different methods. It is clearly shown that the agreement on the temperature distribution is very good, and also fairly good for stresses, using either continuum or discrete methods. However, great discrepancy is observed for water in flux into the tunnel. The dominant reason for this discrepancy is the impact of alternative assumptions of fracture connectivity and how it relates to the macroscopic permeability in fractured crystalline rocks, an important lesson learned for the following phases of DECOVALEX research.

4.2. *FEBEX full-scale heater test (DECOVALEX III)*

The international FEBEX heater test[25,26] was a major modeling task in DECOVALEX III. The FEBEX project was conducted by ENRESA, Spain, with financial support from the European Commission. ENRESA provided to DECOVALEX modeling teams a vast data set covering the first three years of the heating period.

The FEBEX tunnel was excavated in the granite rock at the Grimsel Test Site (Fig. 8), an underground laboratory in Switzerland, operated by the Swiss waste management organization NAGRA. The experiment was based on the Spanish reference concept of deep geological storage in crystalline host rock, in which steel canisters containing conditioned waste are placed along the axis of horizontal galleries, and an engineered barrier of bentonite is placed in the annular space between them. In the FEBEX in situ test, the waste canisters were represented by two cylindrical heaters.

After emplacement of heaters and bentonite blocks and start of the first heating phase in 1997, water began flowing from the granite host rock towards the bentonite, which initially had low saturation. Because the thermal and the hydraulic gradient are in opposite directions, the flow of water and the transport of heat occurred in opposite directions. The thermal gradient caused diffusive vapor transport away from the heater while capillary forces caused water to flow towards the heater. The resulting change in water content led to bentonite shrinkage on the hot dry side (near the heater) and swelling on the cooler wet side (near the bentonite-rock interface), which in turn led to local changes in the stress state of the bentonite and the host rock.

A modeling exercise aimed at predicting the heater test behavior was divided into three parts. In Part A, predictions for both the total water inflow to the tunnel, as well as the water pressure change induced by the boring of the tunnel, were required from the research teams. Part B required predictions of local field variables—such as temperature, relative humidity, stress, and displacement—at selected points in the bentonite barrier. Part C asked for predictions of temperature, stress, water pressure, and displacement at selected points in the host rock. Altogether, ten research teams performed modeling of the test.

Reasonably good agreement was obtained between the predictions and measured results on almost all comparison variables with the coupling mechanisms properly considered in numerical models, especially when the models were calibrated with measured data. Predicting the behavior of the buffer under the combined heating and wetting actions requires a fully coupled THM formulation, which incorporates all the necessary physical processes controlling the bentonite behavior. Only a partial set of codes could offer the required features. The heating of the rock resulted in a significant increase in rock stresses in the vicinity of the FEBEX tunnel. However, water pressures remained essentially unchanged. The relatively high rock permeability explains the absence of significant pore-water pressure transients. Only one of the participating modeling teams was capable of achieving a consistent prediction of all the measured variables in the rock: temperature, water pressure, rock stress, and radial displacement.

Particularly relevant to predicting the early stages of heating was the inclusion of vapor transport as well as accounting for water phase changes. Codes incorporating these features were capable of making good predictions. It should be added that the FEBEX in situ test benefits from comprehensive experimental information on compacted bentonite properties, derived from a large variety of laboratory tests on samples and on small-scale hydration and heating cells.

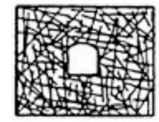
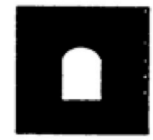
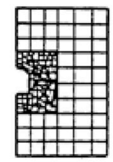
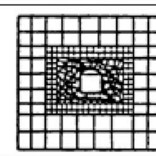
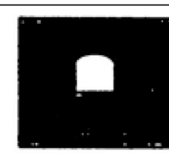
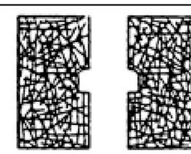
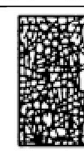
AEA (NAPSAC code, DFN model) Complete and explicit representation of 6580 fractures by DFN method, without heat and rock deformation, but with analytical model for stress approximation.	
CEA/DMT (CASTEM 2000 code, FEM model) Equivalent continuum approach with FEM method (1344 elements, 4216 nodes), homogenization (scale 25 x 25 meters) by Crack Tensor theory [24].	
CNWRA (UDEC code, DEM model) Vertical symmetry and simplified fracture network with 295 fractures, 337 blocks, 1540 finite difference elements, and 10853 nodes. A small inner region with random fractures and lager outer region with regular artificial fractures.	
ITASCA (FLAC code, FDM model) Equivalent continuum approach with FDM (735 finite difference elements and 792 nodes) without formal homogenization. Vertical symmetry and inhomogeneous permeability.	
INERIS (UDEC code, DEM model) Simplified fracture network with inner region of random fractures and outer regions of regular artificial fractures (564 fractures, 677 blocks, 24391 finite difference elements, and 16791 nodes).	
KPH (THAMES code, FEM model) Equivalent continuum approach with FEM method (674 elements, 2127 nodes). Homogenization (scale 10 X 10 meters) by Crack Tensor theory [24]. Heat convection considered.	
NGI (UDEC code, DEM model) Two model of vertical symmetry (one left half and one right half) with simplified fracture network without heating, about 512 fractures, 510 blocks, and 1580 finite difference elements.	
VTT (UDEC code, DEM model) Vertical symmetry (left half) with simplified fracture network, 814 fractures, 496 blocks, 1308 finite difference elements, and 2222 nodes.	

Fig. 5. Different teams, model representations and simplifications for BMT3 (Figure adapted from Stephansson et al.[23]; See Oda[24] for information on equivalent continuum approach with FEM method).

Modeling the FEBEX experiment was a progressive learning process for the teams, a process involving blind prediction and calibration cycles. Some of the physical explanations found for specific measurements (e.g. the development of pore water pressures in the granite when the FEBEX tunnel was excavated) and the progressive improvement of THM codes were highlights of this process. It turned out that a true “blind” prediction was difficult to make even if a highly controlled and documented case (such as FEBEX) was chosen for comparison exercises; nonetheless, such blind comparisons continue to be attempted in the DECOVALEX Project as it is the best test of a model's predictive capabilities, if hard to perform in practice. As predictive modeling improves with the release of additional data, whether or not the relevant coupling mechanisms are properly considered in modeling the FEBEX experiment is a key issue. These mechanisms may or may not be readily identified at the early stage of modeling but can be realized with continued cooperative investigations among the teams.

The DECOVALEX study of the FEBEX experiment represented a major advance in knowledge of the coupled processes in a rock-bentonite-heater system, for all the project participants as well as the broader scientific community. The detailed comparisons of model results with measured data led to new insights into physical explanations for specific measurements (such as the evolution of pore-water pressures in the granite when the FEBEX tunnel was being excavated). More detailed descriptions of the work and achievements, and outstanding issues, can be found in Refs. [25–27]

It is worth noting that in 2002, after about 5 years of heating, a partial dismantling and sampling of the bentonite was carried out (FEBEX II), removing Heater 1 and much of the associated bentonite buffer. Heater 2 on the other hand kept operating for another 13 years, which makes FEBEX the longest running experiment of its scale. In August 2015, the FEBEX-DP project completed dismantling and sampling of Heater 2 and associated bentonite. One of the tasks in the current DECOVALEX-2019 phase revisits the FEBEX experiment and studies the new data, with a particular focus on bentonite heterogeneity

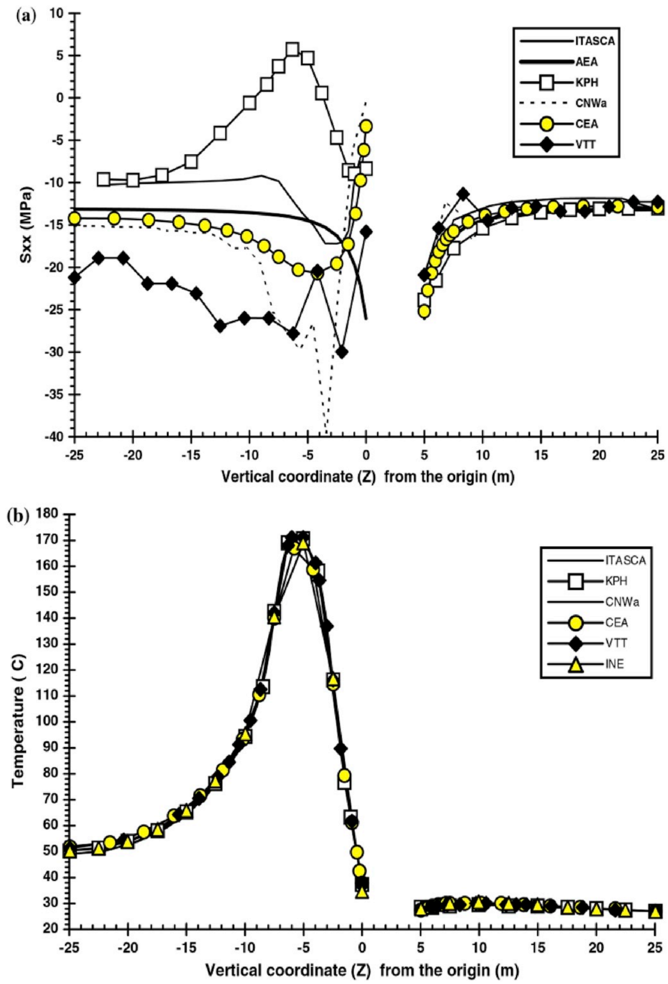


Fig. 6. (a) Horizontal stress (Sxx) along vertical profile across tunnel center at t = 4 years. (b) Temperature along vertical profile across tunnel center at t = 4 years (Adapted from Stephansson et al.[23]).

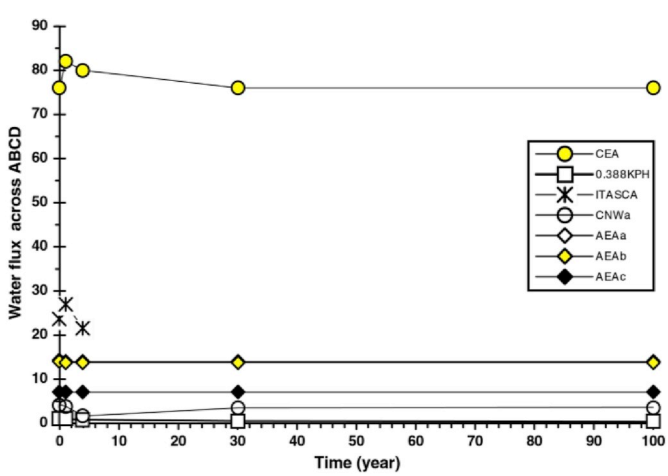


Fig. 7. Water flux ($\times 10^{-8}\,m^3/s$) across the tunnel perimeter as a function of time (Adapted from Stephansson et al.[23]).

evolution, attempting to build on much of the work that was performed in DECOVALEX III.

4.3. Ventilation experiment in Opalinus Clay (DECOVALEX-2011)

The Mont Terri URL is located near a security gallery of a motorway tunnel in northern Switzerland.[28] It is at a depth of about 400 m in Opalinus Clay, which is a stiff layered Mesozoic clay of marine origin. After the excavation of niches in 1996, a new gallery was excavated in 1998, followed by a micro-tunnel of 1.3 m in diameter in early 1999. The ventilation experiment (VE) took place in a sealed 10 m long section of this micro-tunnel (Fig. 9). The experiment consisted of hydraulically "stressing" the host rock by blowing high and low relative humidity air through the sealed section and observing the hydro-mechanical-chemical response.[29] This controlled period lasted approximately 4 years until the end of 2006 and was intended to provoke the kind of extreme humidity conditions that might occur during the repository construction process. By being able to model the complex hydro-mechanical-chemical interactions during this period it was intended that confidence could be built in models to predict the condition of tunnels prior to waste emplacement.

The VE modeling task (part of DECOVALEX-2011) involved building research team expertise through modeling a laboratory drying experiment[29,30] and then progressing onto the field experiment in a piecewise manner, first considering the hydro-mechanical, then non-reactive, and finally reactive geochemical observations. A key requirement of the task specification was a blind prediction of the hydro-mechanical response. This was particularly challenging because evidence from the tunnel showed that the airflow was not sufficiently high to ensure that the applied relative humidity was uniform throughout the tunnel.[30] Therefore, for a genuine prediction, a physics-based representation of the interaction between the tunnel air, injector and host rock was required. Teams adopted different approaches, ranging from calibrated empirical methods to fully coupled abstracted representations of air and vapor migration in the tunnel.[30] It was not found necessary to resort to full CFD (computational fluid dynamics) analysis of airflow in the tunnel, because classical dimensionless analysis indicated simple air flow conditions were likely to dominate. In all cases, good hydro-mechanical responses were obtained by the teams (Figs. 10 and 11).

Modeling of the chloride build-up close to the tunnel as the result of evaporation in the host rock and at the tunnel surface, with resulting back-diffusion into the host rock, was also well-captured using physically plausible parameterization when including the concept of a distinct chloride porosity (Fig. 12). Osmotic water flow effects were not found to be significant in this case and could be safely neglected.[31] One team was able to construct a fully-coupled geochemical representation of the tunnel system, including redox effects and produce good calibrations to observed sulphate concentrations into the tunnel wall.

A key conclusion of this work was that while it was possible to represent the hydro-mechanical evolution of the system without explicit consideration of the water vapor phase (largely by adjusting the water relative permeability functions to give the same net resultant permeability), producing convincing models for the chemical transport component of the analysis was difficult without water vapor. This is not in itself surprising, but it does illustrate that for some modeling applications simplifications can be made to the model formulations if the acceptable bounds of those simplifications are understood, whereas for other applications these simplifications are not acceptable.

4.4. THMC processes in a single fracture (DECOVALEX-2015)

As part of DECOVALEX-2015, a task was conducted to examine the fundamental thermal-hydraulic-mechanical-chemical (THMC) behavior of single fractures at the laboratory scale.[32,33] The experimental work of Yasuhara et al.[34,35] was used wherein artificial single fractures in novaculite (one experiment) and granite (three experiments) were subject to a mechanical confining pressure, variable fluid flows, and different applied temperatures. Differential pressures across the samples were measured to determine permeability and hence hydraulic aperture evolution, while at the same time the chemical composition of the outflows was continually sampled (Fig. 13). For the novaculite

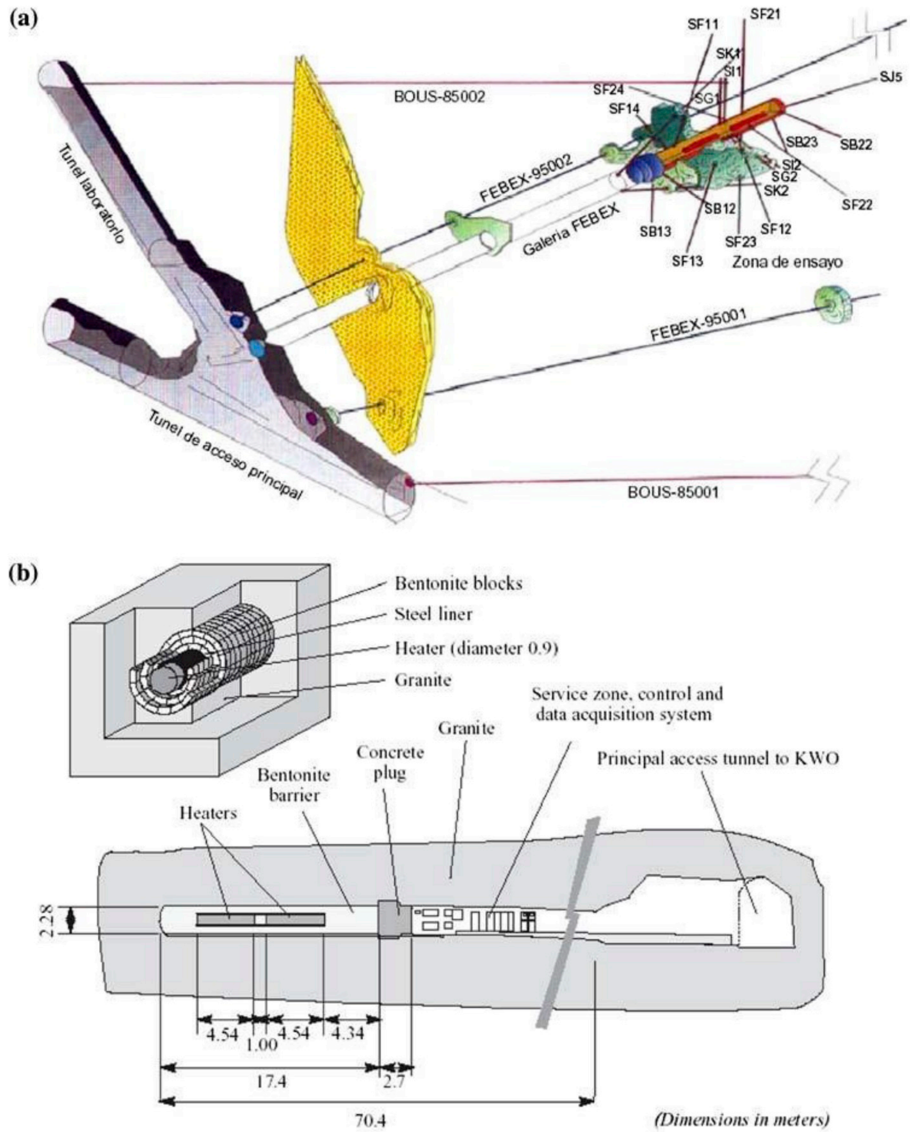


Fig. 8. General scheme of the FEBEX test: (a) 3D perspective; (b) Plan View (Adapted from Alonso et al.[25]).

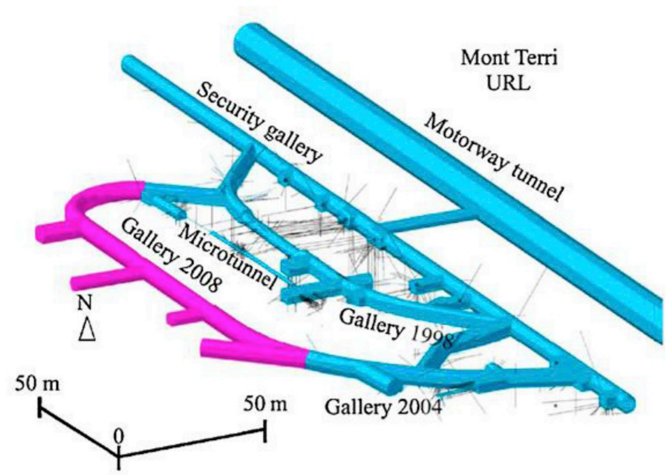


Fig. 9. 3D perspective view of the Mont Terri URL (as of 2008) – the VE experiment was performed in the microtunnel (From Garitte et al.[29]).

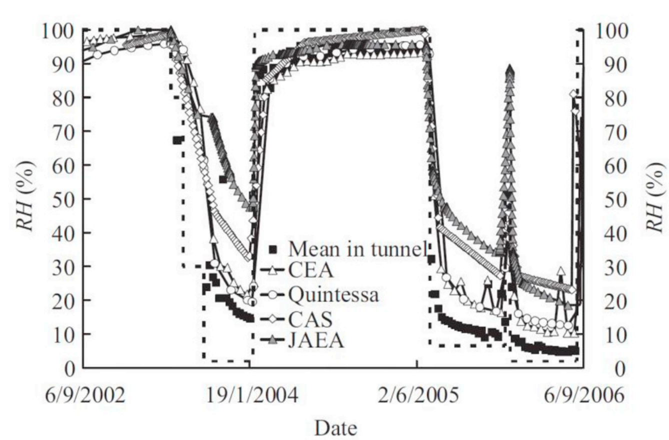


Fig. 10. Comparison of average relative humidity in the tunnel with the calculations performed by the four research teams – dotted line shows the applied relative humidity to the tunnel for the inflowing air (From Garitte et al.[29]).

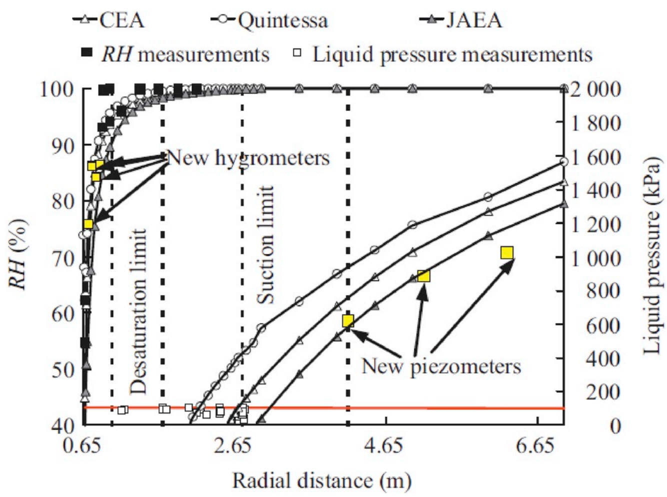


Fig. 11. Measured and predicted liquid pressures and relative humidities (4 October 2006) (From Garitte et al.[29]).

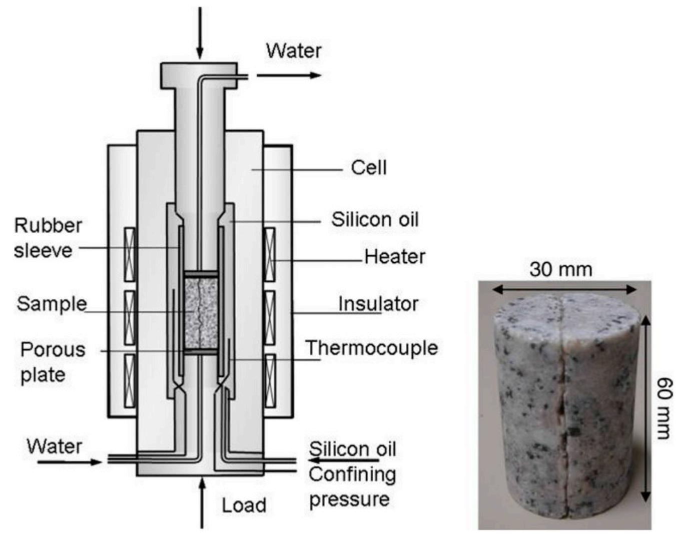


Fig. 13. Schematic illustration of the granite sample test rig (left) and one of the fractured samples (right) (From Yasuhara et al.[35]).

experiments, the topography of the fracture surfaces (Fig. 14) was characterized using a high-resolution laser profilometer, and post-experimental characterization of the aperture was performed using a Wood's metal fracture cast. The objective of the modeling task was to increase the fundamental understanding of micro-scale processes near fracture asperities and use this knowledge to predict the long-term permeability evolution of rock fractures in the near field of repository tunnels.

Six research teams participated in the project and a wide range of numerical approaches was used, including 2D and 3D high resolution coupled thermal-hydraulic-mechanical-chemical (THMC) models. Homogenized "single compartment" models of the fracture were also applied, in an attempt to upscale the processes so that they could be used in larger fracture network studies or in effective continuum models. Particular attention was given to the competing roles of aqueous geochemistry, pressure solution, stress corrosion and pure mechanics in order to reproduce the experimental observations. The definition of the fracture surfaces (and indirectly, aperture) was a particularly intense area of investigation, with a diverse range of statistical approaches developed and applied.[32,33] Acknowledging the complexity of some aspects of the modeling, especially the aqueous geochemistry, simple test cases were used throughout the task to build confidence in the outputs of the different simulation stages.

The resulting models were all able to replicate the key features of the experiments, including the observed fracture closing and opening for the novaculite test (Fig. 15) despite the very different approaches taken by the teams, especially with regards simulating the coupled processes acting on stressed asperity contacts or modeling aqueous geochemistry (Fig. 16). A series of open issues were identified from the study. For example, in order to match observations, all the models relied on very large and temperature-dependent increases in some key parameters, most notably the mineral dissolution rates. Furthermore, the models could be adjusted to better reflect the experimental results

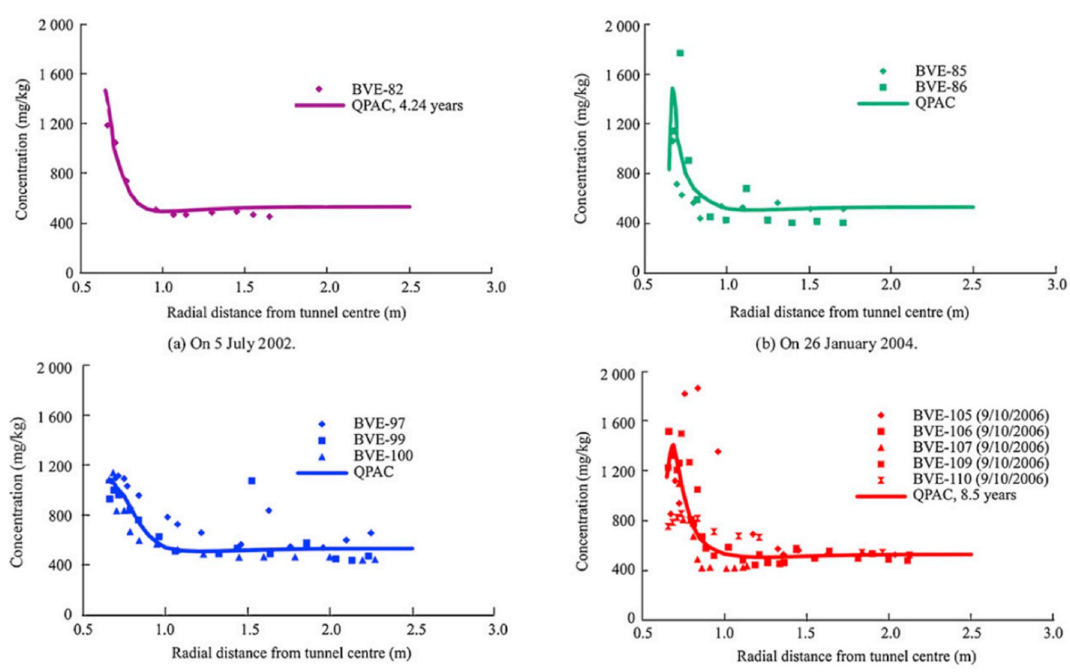


Fig. 12. Example chloride concentration output, showing the results at four different sampling times for the Quintessa team using QPAC (From Bond et al.[31]).

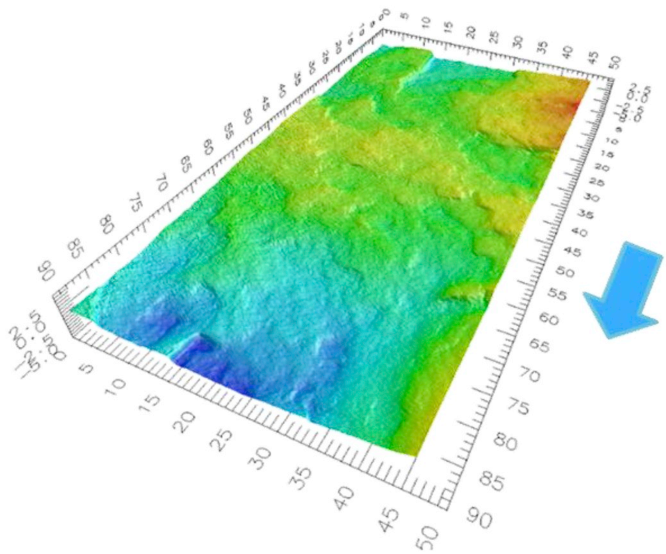


Fig. 14. Surface topography of the novaculite fracture, data presented in Ref. [34] Arrow shows dominant flow direction (Adapted from Bond et al.[32]).

in a self-consistent manner by enhancing (or excluding) different competing processes, such as stress corrosion and rock-matrix diffusion, and it was not possible to quantitatively distinguish which processes were controlling the observed behavior. This task therefore demonstrated that while self-consistent models of such systems are possible to construct, fundamental uncertainties in the underlying physics and chemistry meant that there is no preferable model or models, and thus there was a clear need for well-designed targeted experiments to isolate the relative contribution of the different identified processes.

4.5. SEALEX experiment (DECOVALEX-2015)

The SEALEX experiments comprised a series of field investigations at the Tournemire URL in the south of France.[36] Run by the Institute de Radioprotection et de Sûreté Nucléaire (IRSN), the purpose of the SEALEX experiments was to investigate the performance (in terms of various hydraulic and mechanical properties) of different sealing materials for waste emplacement tunnels during and after the rehydration process. Clay-based swelling core seals were emplaced in 60 cm diameter horizontal deposition holes in the Tournemire argillite, an indurated low-permeability clay. A novel experimental design allowed to impose a constant fluid pressure (or to measure water flux in a later stage) and a watertight seal at both ends of the core seals, provided tight mechanical confinement to ensure a volume-controlled condition along the axial direction during the tests, and featured sophisticated intra-core instrumentation to measure the transient hydro-mechanical (HM) conditions based on wireless instrumentation. The particular experiment for consideration in this task consisted of a seal core made with a 70:30 MX-80 bentonite-sand mixture.

The purpose of the SEALEX modeling task was to develop an understanding of the evolution of performance of clay-based sealing systems and to assist in the interpretation of the experimental data. The task sequence followed what is a typical approach for DECOVALEX tasks, working through a sequence of modeling steps of increasing complexity. An initial modeling step involved laboratory tests on samples with a range of bentonite-sand mixture densities, including oedometer tests and a 1D infiltration test. All the research teams successfully developed models that could replicate the key laboratory observations,[37,38] but there were some key divergences in the approaches used. Constitutive models ranged from direct use of the Barcelona Basic Model for bentonite, to novel models for the plastic response of sealing materials, and finally to relatively simple non-linear elastic models.[37,38]

These models were then applied "blind" to a 1/10th scale SEALEX mockup experiment conducted in the laboratory which included the annular "void" which is also present at the field scale (see Fig. 17). Blind comparisons were only attempted by one of the six teams but the results were good given various uncertainties in the transition from the other laboratory data, specifically a lack of data at lower clay dry densities.[38] The blind prediction gave important insights into the behavior of the constitutive models and was a useful process in the development of the final models. As teams calibrated their models to the 1/10th scale mockup experiment, considerable variation was seen in the treatment of the annular "void" with some teams treating it as a gel of variable stiffness and others using complex boundary conditions coupled with the water inflow rate to approximate the observed behavior. Good calibrated models were obtained in all cases.[37,38]

The final modeling step was simulation of the full bentonite core "in situ" experiment. Unlike the 1/10th mockup experiment, measurements of internal relative humidity and radial stresses were available. The additional data revealed a much more complicated evolution than that shown by the laboratory scale experiments, in part caused by the

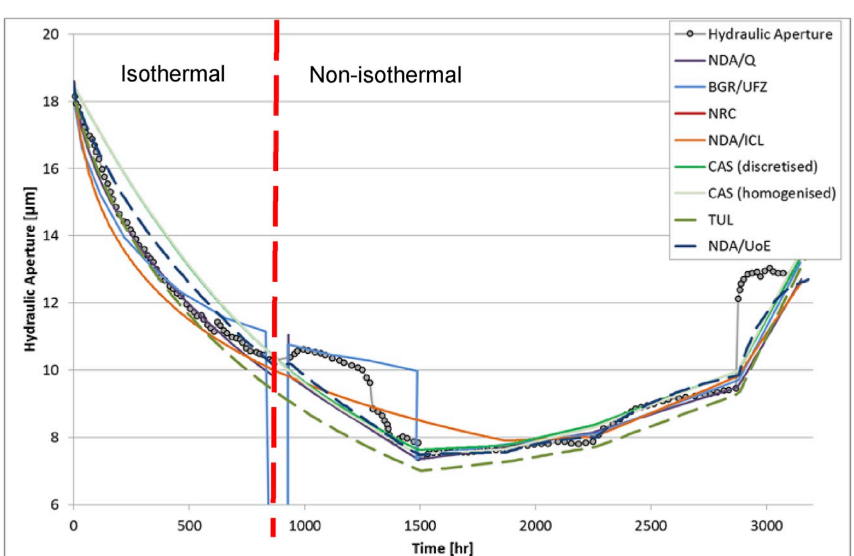


Fig. 15. Comparison of modelled versus observed hydraulic aperture for the novaculite (interpreted using the cubic law from the measured pressure differential as per Yasuhara et al.[34]). Isothermal and non-isothermal parts of the experiment are highlighted (Adapted from Bond et al.[32]).

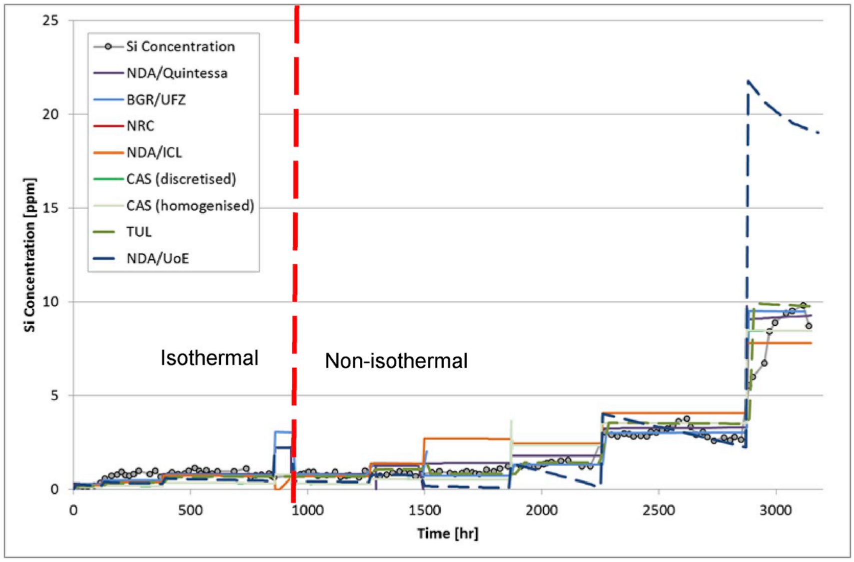


Fig. 16. Comparison of modelled versus observed Si ion concentration in the effluent (ppm) for the novaculite. Isothermal and non-isothermal parts of the experiment are highlighted (Adapted from Bond et al.[32]).

complex interactions of the seal core with the surrounding host rock and the tunnel access gallery. Considerable effort was placed on interpreting the experiments and obtaining good modeling results in most cases, although stress interpretation remained a challenge (Fig. 18).

In performing this exercise, a key divergence between teams was seen in the philosophy of calibrating across all the available experiments at different scales. Some teams attempted to adopt a single model that used a common parameterization (frequently with a strong dry density dependence) and hence had a less good experiment-specific fit, while others chose to calibrate specifically to each experiment and compare variation in input parameters between experiments. Both approaches have value, but there was a clear drive from the project to move towards internal self-consistency in the produced models as these are those that will be more robust for wider application and true prediction. Another major discrepancy was seen in the use on non-linear elastic constitutive models versus full plastic models. It was clear that it would not be possible to fit all the experimental data without some element of mechanical plasticity: however, the larger-scale experiments could be calibrated well using simplified representations. This

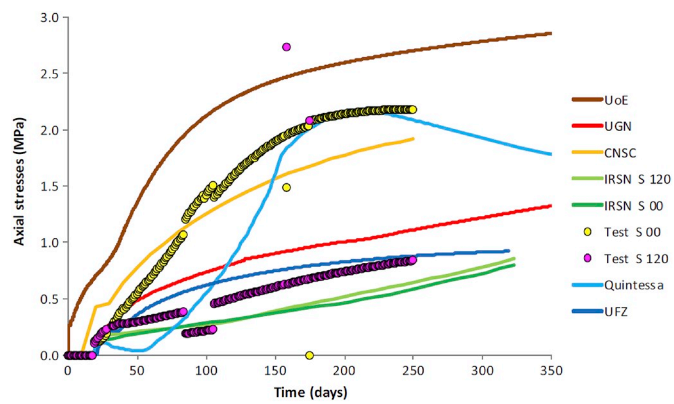


Fig. 18. Comparison of modelled and measured axial stresses for the PT-A1 experiment (From Millard et al.[38]).

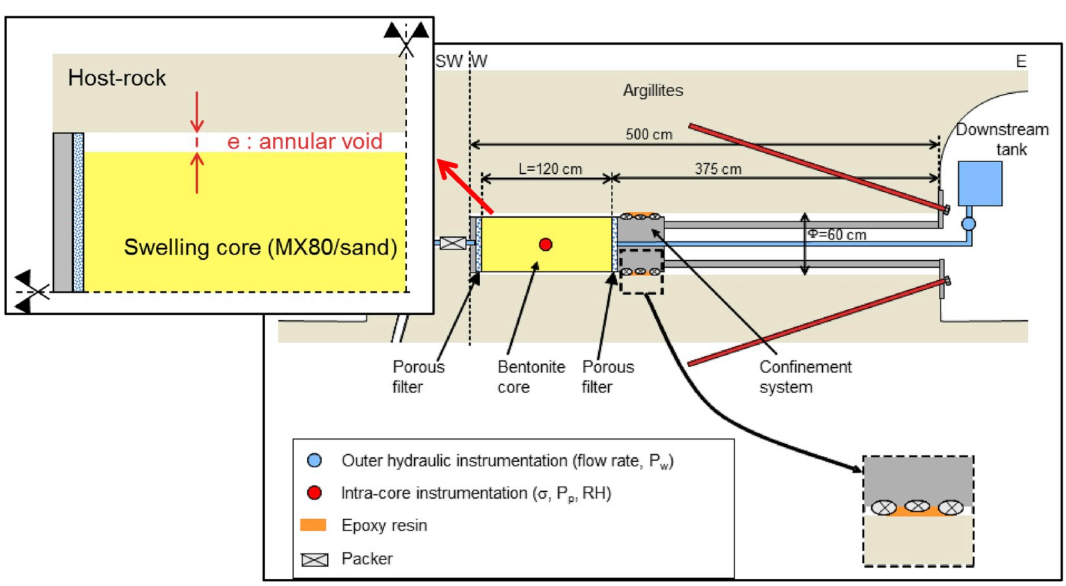


Fig. 17. Schematic illustration of the experimental arrangement in SEALEX Experiment (Adapted from Millard et al.[38] and Barnichon et al.[36]).

observation reinforces the point that a wide range of different model formulations can be useful in simulating a particular set of experiments, but the domain of their applicability needs to be well-understood if they are to be deployed successfully outside of the data, conditions, or scale to which they have been applied and tested.

5. An overview of ongoing tasks in the DECOVALEX project

Here we present three ongoing tasks selected from the current DECOVALEX-2019 phase. As the participating modeling teams are in the middle of conducting a comparative assessment of methods and results, we focus here less on describing the detailed approaches and findings; rather, we intend to illustrate the continued relevance of the DECOVALEX approach to tackling important science questions related to the geological disposal of radioactive waste and spent nuclear fuel as well as other subsurface engineering applications.

5.1. Gas transport in low-permeability clay-based materials

Gas migration in clay-based buffer materials (and clay rocks) has been the subject of a number of international research programs in the field of nuclear waste disposal, including both laboratory scale and in situ experiments.[39–41] A number of model approaches have been proposed for the analysis of the experimental results and for the prediction of gas release scenarios from geological repositories in the context of long-term safety assessment. However, the predictive capability of the gas transport models is yet limited, indicating that basic mechanisms of gas transport in bentonite are not understood in sufficient detail to provide the ground for robust conceptual and quantitative models.

In several repository concepts pursued worldwide, corrosion of metallic materials under anoxic conditions will lead to the formation of hydrogen. Radioactive decay of the waste and radiolysis of water are additional source terms. If the rate of gas produced exceeds the rate of gas transport and dissolution within the pores of the barrier or host rock, a discrete gas phase will form. Gas will continue to accumulate until its pressure becomes sufficiently large for it to enter the surrounding material and migrate away from the waste package, via one of four potential mechanisms as follows (Fig. 19): (1) gas movement by dissolution and subsequent diffusion and entrained advection via migration of the solvent fluid; (2) gas flow in the original porosity of the fabric, commonly referred to as visco-capillary (or two-phase) flow; (3) gas flow along localized dilatant pathways, with potential coupling to the local stress field; and (4) gas fracturing of the buffer material or clay rock similar to that performed during hydrocarbon stimulation exercises.[42,43]

Previous studies on gas migration in clay-based materials[39,44] indicate that classic continuum concepts of porous medium two-phase flow may not be adequate, depending on the scale of the processes and resolution of the numerical model. However, the details of the dilatant mechanisms controlling gas entry, flow and pathway sealing are unclear. As such, development of new and novel numerical representations for the quantitative treatment of gas in clay-based repository systems therefore required, a research need at the center of Task A of the ongoing DECOVALEX phase.[42] The purpose of this task is to better understand the fundamental processes governing the advective movement of gas in low permeability clay barrier materials.[42] Special attention is given to the mechanisms controlling factors such as gas entry and flow, as well as pathway stability and sealing as a function of time, which will impact long-term barrier performance.

To perform this task, data sets on pressure, flow rate, and stress measurements from a series of gas flow tests performed on initially saturated samples have been made available to project participants. These long-term tests, performed under carefully controlled laboratory conditions at the British Geological Survey (BGS), provide detailed data with which to examine gas migration behavior under steady state conditions. As such, a number of test geometries have been used, ranging in complexity from relatively simple one-dimensional flow tests on bentonite to triaxial tests performed on natural samples of COx claystone. To gain insights into the movement of gas through these materials, the laboratory data are used to guide and benchmark numerical model development in an iterative process, increasing in model complexity from one test stage to the next.[42] Fig. 20 shows the pressure vessel used at BGS for monitoring of the evolution of pressure and stress at different locations along of a cylindrical bentonite sample, as well as inflow and outflow rates through filters at both ends of the sample. The first modeling activity in Task A relates to a gas flow test through MX-80 bentonite, with boundary conditions chosen such that the main flow direction is along the axis of the cylinder.

Modeling approaches developed by eight participating modeling teams are tested against the laboratory data, in a staged manner, building up in complexity (both in terms of the experimental and modeling approaches). As the modeling activities are still ongoing, we are not presenting any details on modeling results. Rather, we like to demonstrate here the breadth of the simulation approaches tested in Task A. Table 1 provides an overview of the eleven modeling approaches pursued by eight research teams. There are essentially three main strategies each based on a different interpretation of the underlying physics: (1) A variety of teams are pursuing two-phase continuum methods coupled to a range of alternative descriptions of mechanical deformation (elastic, viscoelastic, elastoplastic, damage). (2) Two teams attempt to explain the observed behavior with two-phase continuum models with preferential pathways, in one case assuming separate conduits for water and gas, in the other case accounting for embedded micro-fractures acting as gas conduits. (3) Finally, two teams are applying discrete pathway approaches: (a) a distinct element model to explicitly model the opening of grain boundaries for dilatant gas migration based on a fracture mechanics formulation, and (b) a bubble transport model on the chaotic nonlinear dynamic aspects of gas

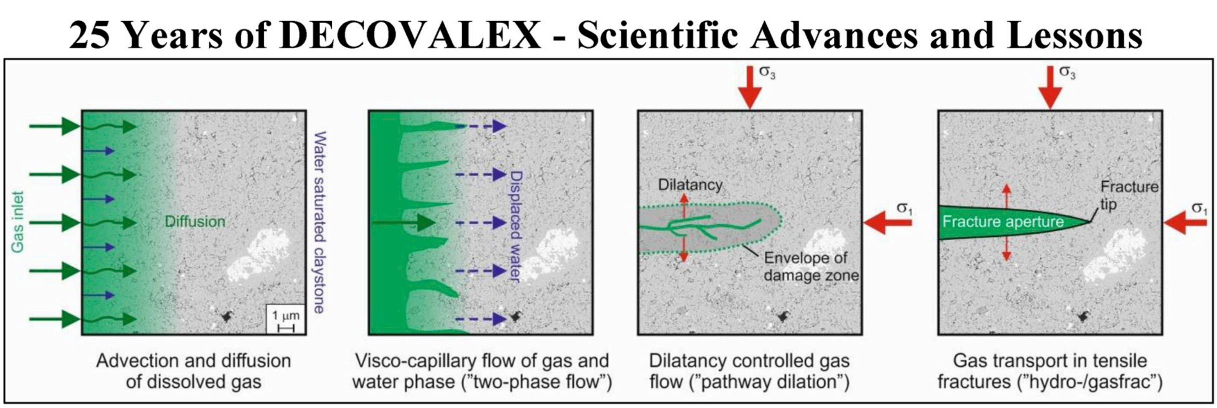


Fig. 19. Conceptual models for gas migration in low-permeability clays (Based on Harrington and Hoseman[44]).

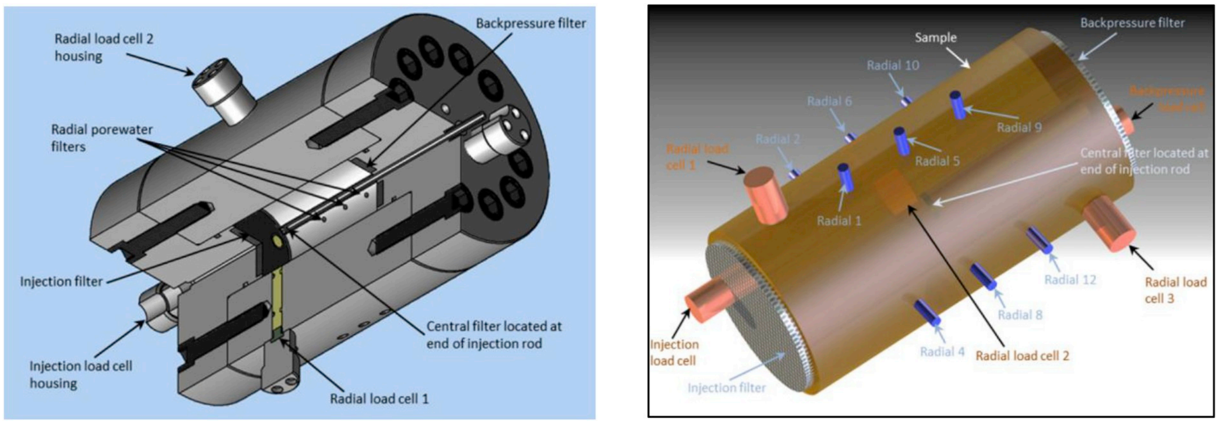


Fig. 20. Gas injection tests in compacted bentonite. Left: Cut-away diagram of the pressure vessel showing the apparatus components and instrumentation. Right: image of the sample showing the relative positions of the load cells and pore pressure filters (From Harrington[42]).

migration. It is anticipated that by the end of the current DECOVALEX phase in December 2019, this task will provide valuable tested predictive tools to assess the impact of gas flow on barrier and host materials, providing information which can be used to support future repository design.

5.2. Upscaling THM processes observed in various heater experiments

The purpose of this task (Task E of the ongoing DECOVALEX-2019 phase) is upscaling THM models using laboratory data (cm scale) applied to small size experiments (a few meters) to real scale emplacement cells (tens of meters) all the way to scale of a waste repository (kilometers). The task, aligned with the French repository design, assumes that waste canisters will be placed horizontally in a series of parallel micro-tunnels drilled from access drifts, each microtunnel about 80 m long and 0.7 m in diameter, in Callovo-Oxfordian claystone (COx) formation (Fig. 21). A comprehensive research program was conducted by the French radioactive waste management agency ANDRA in their underground research laboratory near Bure to investigate the THM response of the COx to thermal loading from parallel microtunnels, through laboratory and in situ experiments. The in situ experimental program consists of a step-by-step approach ranging from small-scale heating boreholes (TED experiment) to full-scale experiments (ALC experiment) (Fig. 22). Results from these heater experiments, as well as data from large-scale site characterization including geophysical measurements over the repository footprint) have been provided to DECOVALEX.

Like in most other DECOVALEX tasks, the modeling program is organized in several sub-tasks, in this case including a benchmark test, an interpretive exercise, a blind prediction, and a large-scale application.[45] In a first step, the models used are benchmarked against 3D analytical solutions to validate the correctness of code implementation considering THM processes. The second step consists of interpretative modeling of the small-scale in situ heating experiment (TED) realized in ANDRA's URL. The TED experiment, which started in 2010 and ended in 2013, involved three small heaters directly placed into narrow boreholes parallel to each other at a distance of about 2.7 m. The third step involves the interpretation and modeling of a full-scale heating experiment based on results from model calibrations at the smaller scale (TED experiment). ALC is an ongoing in situ test designed as a realistic representation of a micro-tunnel used for waste emplacement using very similar dimensions and designs to the current concept. The interaction between the tunnel support (steel casing in this case), the EDZ, and the surrounding intact rock is closely investigated through this full-scale scale experiment to assess the effect of the thermal loading on the steel structure. The extent of the behavior of one single emplacement cell relative to the behavior at the repository scale (several parallel emplacement cells) will be approached in a last step as a modeling comparison exercise. Key questions addressed in this final step are (1) how to extrapolate data, processes, and models from URL scale (areal size of 0.1 km^2) to the scale of an entire repository of about 9 km^2, and (2) how to take into account the geological variability as evident from site characterization from the small to the large scale? Fig. 22 illustrates the stepwise modeling sequence with steps of increasing scale and complexity. Six modeling teams from five countries are participating in this task.

5.3. Induced slip of a fault in argillaceous rock

This modeling task evaluates the conditions for slip activation and stability of faults in clay formations and in particular addresses the complex coupling between fault slip, pore pressure, permeability creation, and fluid migration (Task B in the current DECOVALEX phase). The subject is of great importance to many subsurface applications where injection of fluids leads to pore-pressure increase and reduction of effective normal stresses on faults, which in turn can cause fault reactivation. Regarding radioactive waste emplacement, increases in pore pressure could be caused by release of heat from the high-level waste or by the generation of gas due to steel corrosion. The possibility of an increased permeability caused by fault slip and generation of potential pathways in the host rock in an upper sealing formation could be a major risk for the long-term safety of a repository.

The central element of the modeling task is the FS Fault Slip Experiment conducted in 2015 at the Mont Terri URL in Switzerland, which utilized a novel experimental setup for controlled fault slip testing in realistic underground settings at the field scale.[46–48] As shown in Fig. 23, a borehole intersecting a fault was equipped with a newly developed borehole probe consisting of a straddle packer system that can be stepwise pressurized via fluid injection and that contains a three-component extensometer connecting the two packers in the injection chamber. This extensometer is fixed to the borehole wall by hydraulically operated anchors, thus providing a high-resolution and high-frequency device measuring at nano-scale resolution both axial and radial deformations between the upper and lower anchor points. The probe also monitors downhole fluid pressure and flow rate as the fault is slipping, an unprecedented data set for evaluating the transient coupling between fault opening and slip, pore pressure, permeability creation, and fluid migration. Of five injection tests conducted in different boreholes and different intervals at Mont Terri, two tests were selected for modeling within DECOVALEX-2019. The tests provide data for activation of the main fault as well as minor faults/fractures in the fault damage zone, respectively.

As mentioned above, the topic of pressure-induced fault reactivation and seismicity is of relevance to the broader set of subsurface

Table 1
Overview of modeling approaches used in Task A of DECOVALEX-2019.

Team	Formulation	Mechanical deformation	Software	Test geometry	Calibration parameters
BGR/UFZ	multiphase flow model	elasto-plasticity	OpenGeoSys	2D axisym.	Intrinsic permeability, critical pressure
CNSC	two-phase flow model	damage	COMSOL Multiphysics	2D axisym., 3D	Air entry value, maximum intrinsic permeability, damage smoothing parameter, swelling coeff.
KAERI	two-phase flow model	damage	TOUGHMP-FLAC3D	3D	Damage parameters
LBNL	multiphase flow model	elasticity	TOUGH2-FLAC3D	3D	Intrinsic permeability, moisture swelling coeff., stress-perm function
	multiphase flow model	discrete fractures	TOUGH-RBSN	2D plane	Strength and elastic parameter of fractures
SNL	chaotic model	fractures	no specific code	0D	NA
NCU/TP	multiphase flow model	viscoelasticity	In-house	2D plane	Intrinsic permeability, air entry value, viscous parameters
Quintessa/RWM	two-phase flow (separate gas, water paths)	elasticity	QPAC	1D	Capillarity compressibility, capillary spacing, swelling pressure, Biot coefficient
UPC/Andra	two-phase	rigid body	CODE_BRIGHT	3D	Gas relative permeability, intrinsic permeability
	embedded permeability	rigid body	CODE_BRIGHT	3D	Embedded permeability parameters

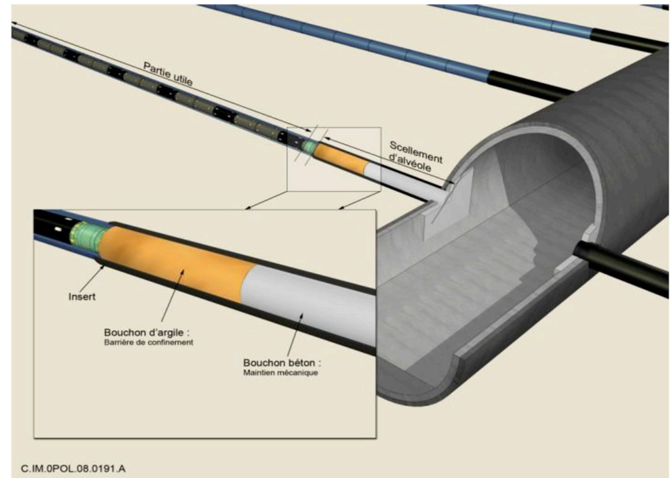


Fig. 21. French design for disposal in argillaceous rock, with waste packages stored in horizontal microtunnels (Adapted from Vitel et al.[45]).

applications; at the same time, issues surrounding fault slip and related permeability creation have not often been a focus of the waste disposal science community. Thus, it made a lot of sense to open up this task to external participation, inviting organizations that have not traditionally part of DECOVALEX. Seven modeling teams from seven countries are currently participating in Task B activities, using a range of methods such as the classical hydro-mechanical continuum models with faults represented as embedded weak planes and the distinct element methods where the rock mass is represented as an assembly of discrete blocks and fault/fractures are viewed as interfaces between distinct bodies.

The modeling task is organized in a stepwise approach. Step 1 comprises benchmark simulations (Fig. 24) to evaluate the activation of a simplified fault plane. This allows for necessary model developments and comparative testing related to modeling of fault activation processes, such as developing and testing new constitutive models for fault hydro-mechanical behavior. Based on a successful simulation of the simplified benchmark, teams are now working on Step 2 conducting interpretative modeling of the observed activation and hydromechanical behavior of a minor fault. Step 3 then will move the teams into a final stage to perform interpretative modeling of the complex activation patterns observed in the main fault at Mont Terri, which resulted in strong shear activation and considerable permeability changes.

6. Concluding remarks and a brief summary of scientific advances under DECOVALEX

As an international cooperative research project, DECOVALEX is probably unique in its longevity and productivity, with no decrease in enthusiasm among the project participants even after 25 years. The current phase of the project, referred to as DECOVALEX-2019, features a record number of tasks (seven) and a near-record number of funding organizations (13). The reason for this enduring success, we believe, is four-fold. First the organization of the cooperative project is simple and effective, allowing the project to adapt itself with scientific advances and with developing research interests of participants. Second, the participants are willing to share data and information from expensive, multi-year field tests and large-scale laboratory experiments, and in some cases, are open to suggestions from DECOVALEX participants to modify the tests and make new measurements. This is obviously very helpful to data-receiving participants who are able to study these data and learn the science behind them, but it is also very helpful to the data-producing participants who benefit from an international group of experts analyzing and simulating their expensive laboratory experiments and field tests from different angles. The insight and scientific knowledge gained in this collaborative setting would not have been possible if one group had studied these data alone. Thirdly, DECOVALEX has

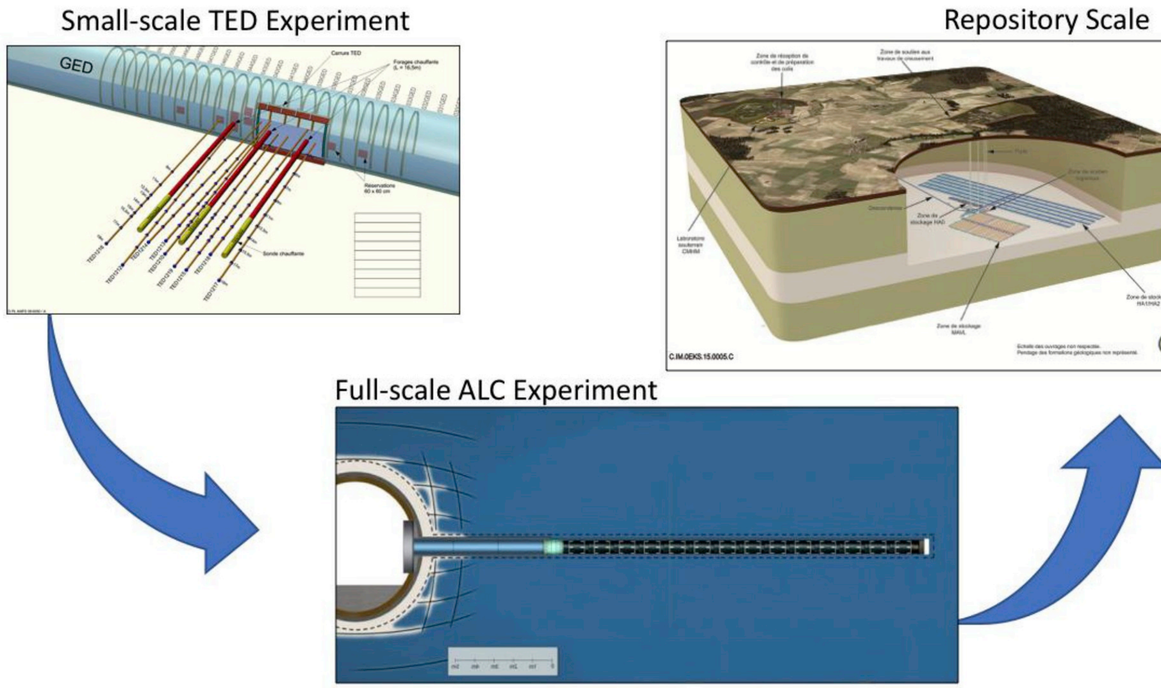


Fig. 22. Schematic showing the workflow from simulating small-scale borehole tests to 1:1 scale heater tests in micro-tunnels to thermal processes in the entire repository. The workflow starts with core-scale experiments, which are not shown here (Adapted from Vitel et al.[45]).

always emphasized publications in reputable peer-reviewed journals and in books and monographs. In this way the project opens its work to review and critique from the scientific community at large which helps to maintain the scientific standard of its research. And, fourthly, the project is carried out through frequent and in-depth discussion meetings among the participants in a mutually supportive atmosphere. It has been a pleasant learning experience for all the participants to enter into the complexity and significance of coupled THM and THMC processes in geological media, and it is a good forum to nurture young graduate students and early-career researchers as well as new research teams to bring them up to speed in coupled processes research.

Over the last 25 years, a number of important advances in coupled THMC research have been made through work in or associated with DECOVALEX. Below we highlight some major accomplishments in

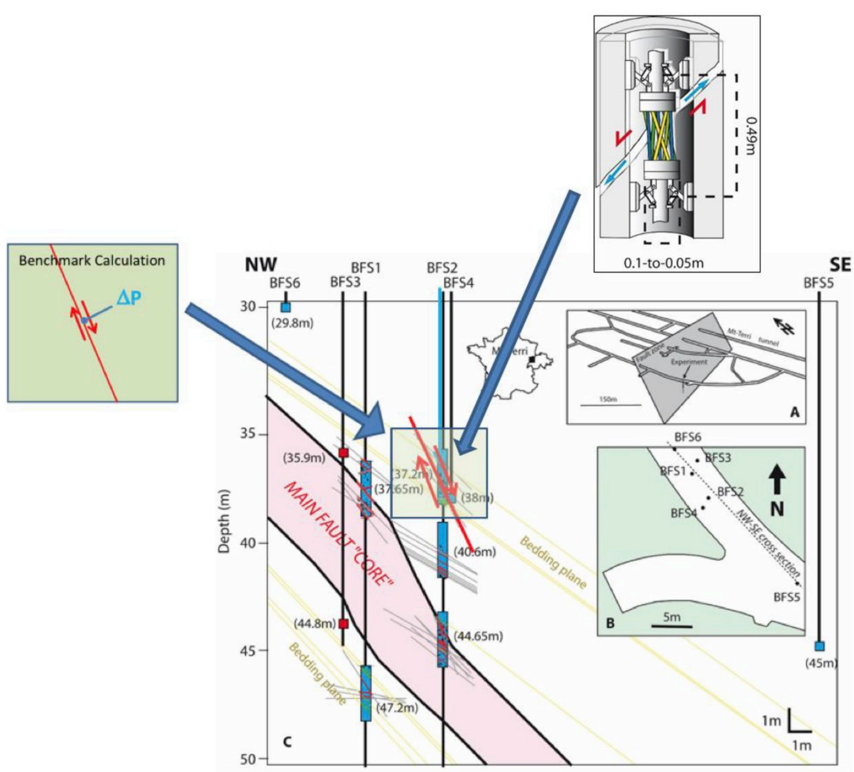


Fig. 23. Schematic figure showing fault at Mont Terri URL with injection and reactivation area (From Guglielmi et al.[48]).

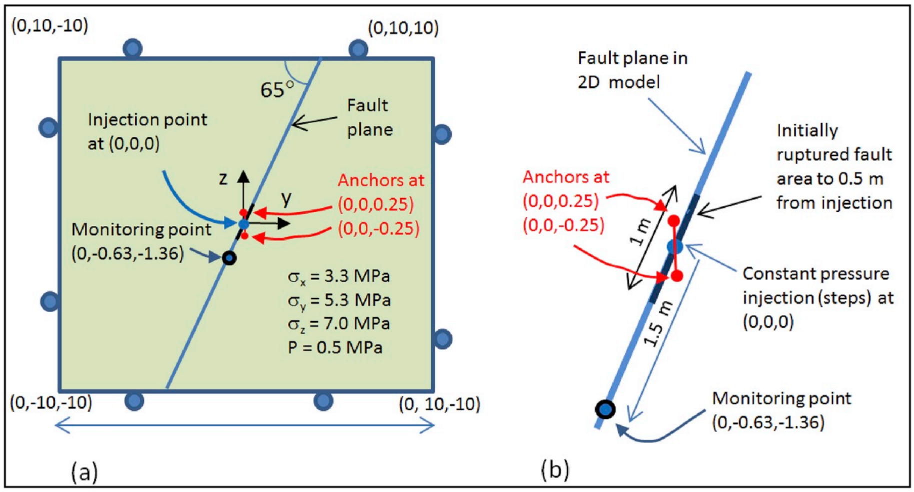


Fig. 24. First modeling step with simplified geometry and defined conditions.

reference to the example tasks introduced in this paper. A more complete view may be obtained from books and journal special issues specifically on DECOVALX results, which are in Appendix B for the convenience of the readers.

- A definitive study of conceptual model uncertainty by a comparative investigation into coupled THM processes in fractured rock through the use of eight different conceptual models (this was presented in Section 4.1; see Fig. 5). Through such a concrete case study, more insight has been gained on this type of uncertainty and its implication for long-term system evolution.
- An in-depth analysis of large complex in-situ experiments studying full-scale THMC processes in different host rocks, demonstrating that the early perturbations from future radioactive waste emplacement can be predicted with good and well-characterized confidence (an example is shown in Section 4.2; see Fig. 8).
- A comprehensive review of coupled THMC processes in the EDZ around subsurface opening for different rock types: crystalline rock, plastic clay, indurated clay, and salt. This helped to stimulate the study of EDZ in several rock types using the same numerical simulator, thus providing enhanced insight into such systems. As an example of a rock-type specific study, the Ventilation Experiment discussed in Section 4.3 (see Fig. 9) explored how wetting and drying cycles in future waste disposal tunnels may affect the EDZ properties in an indurated clay.
- A first systematic examination of the ability of discrete and continuum approaches to predict the micro-scale THMC processes occurring in individual fractures exposed to stress, temperature, and reactions (Section 4.4; Figs. 13 and 14).
- One of the first detailed studies of coupled hydraulic, mechanical and chemical processes in the bentonite barrier and its interaction with the surrounding rock (an example is given in Section 4.5; see Fig. 17). This laid the ground work for many further studies into coupled processes at the bentonite-rock interface.

In addition to in-depth evaluation of coupled processes, the DECOVALEX Project has always been interested in their impact on the long-term safety of a geological repository. For example, one task in DECOVALEX III investigated methods for upscaling the THM properties of a fractured rock mass so that they can be used in large-scale repository performance assessment models. Furthermore, a series of papers were published on the hydromechanical processes in fractured rocks induced by the advancement and retreat of glaciation and its effect on the far-field flow and transport of potential radionuclide leakage from a waste repository to the biosphere. Such studies allowed for establishing clear relationships between coupled processes and overall repository performance.

At the 25-year mark of DECOVALEX, it is useful to look back and review the scientific advances that have emerged from DECOVALEX and the possible reasons behind its longevity and continuing success. Perhaps such a review may point to an effective possible approach to future international collaborative research in geosciences. It will also be interesting to follow the future development of DECOVALEX, as discussions are now underway to plan for the next phase, DECOVALEX-2023. Ultimately, it is the interests and needs of the participating organizations that drive the focus of the project by proposing and selecting the modeling tasks. As a result, the research areas of the DECOVALEX project have always closely mirrored the evolution of scientific interest of the community at large, and we expect this correlation to continue, thereby ensuring continued relevance. It is thus a bit speculative when we make an attempt to identify research trends for future DECOVALEX phases but we shall do it here briefly as a framework and starting point for continuing discussion of new ideas. First, we may expect that some aspects of the project will be broadened to include wider geo-engineering problems facing society, such as geologic carbon sequestration and enhanced geothermal resources development, while retaining a core focus on radioactive waste disposal. Second, in terms of topics for future consideration, it is likely that the engineered barrier system (or 'near-field') will remain a priority for the project. Furthermore, potential host-rocks such as evaporitic and diagenetic salts are likely to regain an interest where there are a wide variety of challenges in both radioactive waste and other subsurface engineering applications (e.g., energy storage). In terms of technologies and approaches, it is expected that DECOVALEX will take advantage of increasingly accessible high-performance computing (HPC) together with robust standard libraries for implementing numerical models in massively parallel environments. The current advances of machine-learning cannot be ignored, and it is likely that some of the techniques being developed will facilitate complementary modeling and data analysis approaches. Ultimately the advances made in the DECOVALEX Project will need to be evaluated by their capability to build confidence in the understanding and modeling coupled processes in geo-engineering projects, with the goal of furthering our ability to robustly evaluate the safety of radioactive waste and other sub-surface engineering applications.

Acknowledgment

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Appendix A. Funding organizations and research teams during the DECOVALEX Project, from 1992 to 2018

Acronym	Funding Organizations	Country	I 1992–1994	II 1995–1999	III 2000–2003	THMC 2004–2007	2011 2008–2011	2015 2012–2015	2019 2016–2019
AECB	Atomic Energy Control Board	Canada		X					
AECL	Atomic Energy of Canada Limited	Canada	X	X					
ANDRA	National Agency for Radioactive Waste Manag.	France	X	X	X				X
BGR	Federal Institute for Geoscienc. and Natural Res.	Germany			X	X		X	X
CAS	China Academy of Sciences, IRSM	China				X	X	X	
CEA	Commisariat a l'Energie Atomique	France	X		X				
CNSC	Canadian Nuclear Safety Commission	Canada			X				X
DOE	Department of Energy	USA			X	X		X	X
EA	Environmental Agency	UK		X					
ENRESA	Empresa Nacional de Residos Radioactivids	Spain		X	X				
ENSI	Swiss Federal Nuclear Safety Inspectorate	Switzerland						X	X
EU	European Union (through Benchpar Project)	Europe			X				
IPSN	Institute de Protection et de Sûreté Nucléaire	France		X					
IRSN	Institute for Protection and Nuclear Safety	France			X	X	X	X	X
JAEA	Japan Atomic Energy Agency	Japan				X	X	X	X
JNC	Japan Nucl. Cycle Developm. Inst. (former PNC)	Japan	X	X	X				
KAERI	Korean Atomic Energy Research Institute	Korea					X	X	X
NIREX	United Kingdom Nirex Ltd	UK	X	X	X				
NRC	Nuclear Regulatory Commission	USA	X		X			X	
NWMO	Nuclear Waste Management Organization	Canada				X			X
OPG	Ontario Power Generation (former OH)	Canada		X	X				
POSIVA	Posiva Oy	Finland					X		
RWM	Radioactive Waste Management	UK					X	X	X
SKB	Swedish Nuclear Fuel and Waste Management	Sweden	X	X	X	X	X		
SKI	Swedish Nuclear Power Inspectorate	Sweden	X	X	X	X			
SSM	Swedish Radiation Safety Authority	Sweden							X
STUK	Radiation and Nuclear Safety Authority	Finland	X	X	X	X			
SÚRAO	Radioactive Waste Repository Authority	Czech Rep.					X	X	X
TaiPower	Taiwan Power Company	Taiwan							X
WHU	Wuhan University	China					X		
Total number of funding organizations per phase			9	12	15	9	9	10	13

Appendix B. DECOVALEX phases, tasks, and major publications

Phase/Time Period	BMT, TC and Task	References to Results
DECOVALEX I 1992–1994	BMT 1: Fractured rock with two orthogonal sets of persistent fractures and a heat source BMT 2: Fractured rock with four discrete fractures and a finite- length heat source BMT 3: Fractured rock with a realistic fracture network of 6580 fractures from Stripa mine data TC 1: Laboratory shear-flow test on rock core sample with a single joint TC 2: Field experiment in fractured rock at Fanay-Augeres, France TC 3: Large-scale laboratory experiment of engineered buffer material (Big-Ben experiment, Japan) TC 4: Laboratory stress flow tests on rock fractures TC 5: Laboratory shear-flow experiment of a rock block with a single joint TC 6: Field experiment of hydraulic injection test on fractures at 356 m depth	Elsevier Book Series Developments in Geotechnical Engineering: Coupled Thermo-Hydro-Mechanical Processes of Fractured Media: Mathematical and Experimental Studies (Volume 791996) Special Issue, International Journal of Rock Mechanics and Mining Sciences (Volume 32, Number 5, 2001).

DECOVALEX II 1995–1999	Task 1: Numerical study of Nirex's Rock Characterization Facility (RCF) shaft excavation at Sellafield, UK Task 2: Numerical study of PNC's in situ THM experiments in Kamaishi Mine, Japan Task 3: Review of the state-of-the-art of the constitutive relations for rock joints Task 4: Current understanding of the coupled THM processes related to design and PA of radioactive waste repositories	Special Issue, International Journal of Rock Mechanics and Mining Sciences (Volume 38, Number 1, 2001).
DECOVALEX III 2000–2003	Task 1: FEBEX (Full-scale engineered barriers experiment in crystalline host rock) Task 2: The Drift Scale Test (DST) at Yucca Mountain BMT 1: Implications of THM coupling on the near-field safety of a nuclear waste repository. BMT 2: Upscaling of the THM properties in a fractured rock mass and its significance for large-scale repository PA BMT 3: The THM responses to a glacial cycle and their potential implications for deep geological disposal of nuclear fuel waste in a fractured crystalline rock mass	Elsevier Geo-Engineering Book Series: Coupled Thermo-Hydro-Mechanical-Chemical Processes in Geo-Systems - Fundamentals, Modeling, Experiments and Applications (Volume 2, 2004) Special Issue, International Journal of Rock Mechanics and Mining Sciences (Volume 42, Number 5–6, 2005).
DECOVALEX THMC 2004–2007	Task A: Influence of near field coupled phenomena on the performance of a spent fuel repository Task B: Understanding and characterizing the excavation damaged zone (EDZ) Task C: Excavation damaged zone (EDZ) in the argillaceous Tournemire Site (France) Task D: Long-term permeability/porosity changes in the EDZ and near field, due to THM and THC processes in volcanic and crystalline-bentonite systems Task E: THM processes associated with long-term climate change: glaciation case study	Special Issue, The DECOVALEX-THMC Project (Safety assessment of nuclear waste repositories), Journal of Environmental Geology (Volume 57, Number 6, 2009).
DECOVALEX 2011 2008–2011	Task A: HM-C processes in argillaceous rocks Task B: TM modeling of fracture initiation and propagation, and rock spalling in rock openings Task C: Assessment of coupled THMC processes in single fractures and fractured rocks	Special Issue on DECOVALEX 2011 - Part 1 and 2, Journal of Rock Mechanics and Geotechnical Engineering (Volume 5, Issues 1 and 2, 2013)
DECOVALEX 2015 2012–2015	Task A: The SEALEX Experiment - HM processes in bentonite-based sealing structures Task B1: THM processes in bentonite buffers and argillaceous host rocks Task B2: The Horonobe EBS experiment - THMC processes in buffer, backfill and host rock Task C1: THMC processes in single fractures of novaculite (micro-crystalline quartz) and granite Task C2: The Bedrichov Tunnel - hydro-chemical interactions in a fractured crystalline rock	Special Issue, Environmental Earth Sciences. Topical Collection: DECOVALEX 2015 ISSN: 1866–6280 (Print) 1866–6299 (Online)
DECOVALEX 2019 2016–2019 (Ongoing at the time of writing this paper)	Task A: Advective gas flow in low permeability sealing materials Task B: Induced slip of a fault in argillaceous rock Task C: Hydro-mechanical-chemical-biological processes during Groundwater Recovery in Crystalline Rock Task D: Hydro-mechanical (HM) and THM interactions in bentonite engineered barriers Task E: Upscaling of heater test modeling results Task F: Fluid inclusion and movement in tight rock Task G: EDZ Evolution - Reliability, feasibility, and significance of measurements of conductivity and transmissivity of the rock mass	

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